LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061116\
Data File : BF087938.D
Acq On : 12 Jun 2016 9:45
Operator : UM/SJ
Sample : H3504-06
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-6

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-BF060716.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	1.736	12	13	22	rVB	235212	367110	9.06%	1.217%
2	1.861	22	24	38	rVB	1914178	3036203	74.96%	10.065%
3	4.970	293	296	302	rVB	86540	108559	2.68%	0.360%
4	5.393	330	333	335	rBV	1784910	1714928	42.34%	5.685%
5	6.433	421	424	426	rVB	1295794	1157269	28.57%	3.836%
6	6.570	433	436	438	rBV	2589360	2797194	69.06%	9.273%
7	6.799	454	456	458	rBV	846677	698135	17.24%	2.314%
8	6.867	460	462	467	rBV	104869	97784	2.41%	0.324%
9	6.959	467	470	472	rBV	2568351	2442285	60.29%	8.096%
10	7.370	502	506	508	rBV	1900497	2135132	52.71%	7.078%
11	7.473	511	515	519	rVV	45611	70733	1.75%	0.234%
12	8.090	566	569	571	rBV	1036244	976055	24.10%	3.236%
13	8.799	629	631	633	rBV	119183	133571	3.30%	0.443%
14	9.165	660	663	666	rBV	2594307	4050565	100.00%	13.428%
15	9.565	695	698	700	rBV	208465	218175	5.39%	0.723%
16	9.839	720	722	725	rBV	1101907	1041222	25.71%	3.452%
17	10.285	757	761	762	rBV2	45138	69171	1.71%	0.229%
18	10.628	788	791	794	rBV2	1581835	2208710	54.53%	7.322%
19	10.754	800	802	806	rVB	62098	79227	1.96%	0.263%
20	11.325	849	852	854	rBV	1135071	1107507	27.34%	3.671%
21	11.371	854	856	863	rVB2	22836	43030	1.06%	0.143%
22	11.565	870	873	876	rVB	75635	97031	2.40%	0.322%
23	11.645	876	880	882	rBV2	24066	41334	1.02%	0.137%
24	12.628	964	966	969	rBV	50468	64364	1.59%	0.213%
25	12.742	974	976	978	rBV	202758	187343	4.63%	0.621%
26	12.811	979	982	985	rVB3	28966	60452	1.49%	0.200%
27	12.914	988	991	993	rBV	2831387	3140363	77.53%	10.410%
28	12.948	993	994	999	rVB	31152	51751	1.28%	0.172%
29	13.440	1036	1037	1039	rBV	103245	113428	2.80%	0.376%
30	13.817	1068	1070	1075	rBV	126552	147956	3.65%	0.490%
31	13.954	1079	1082	1085	rBV	931240	885677	21.87%	2.936%
32	14.731	1148	1150	1155	rVB	26765	41256	1.02%	0.137%
33	14.811	1155	1157	1163	rVB2	33577	63211	1.56%	0.210%
34	15.371	1203	1206	1208	rBV	509755	667248	16.47%	2.212%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061116\
Data File : BF087938.D
Acq On : 12 Jun 2016 9:45
Operator : UM/SJ
Sample : H3504-06
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-6

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-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.417	1208	1210	1214	rVB	29456	52012	1.28%	0.172%

Sum of corrected areas: 30165991

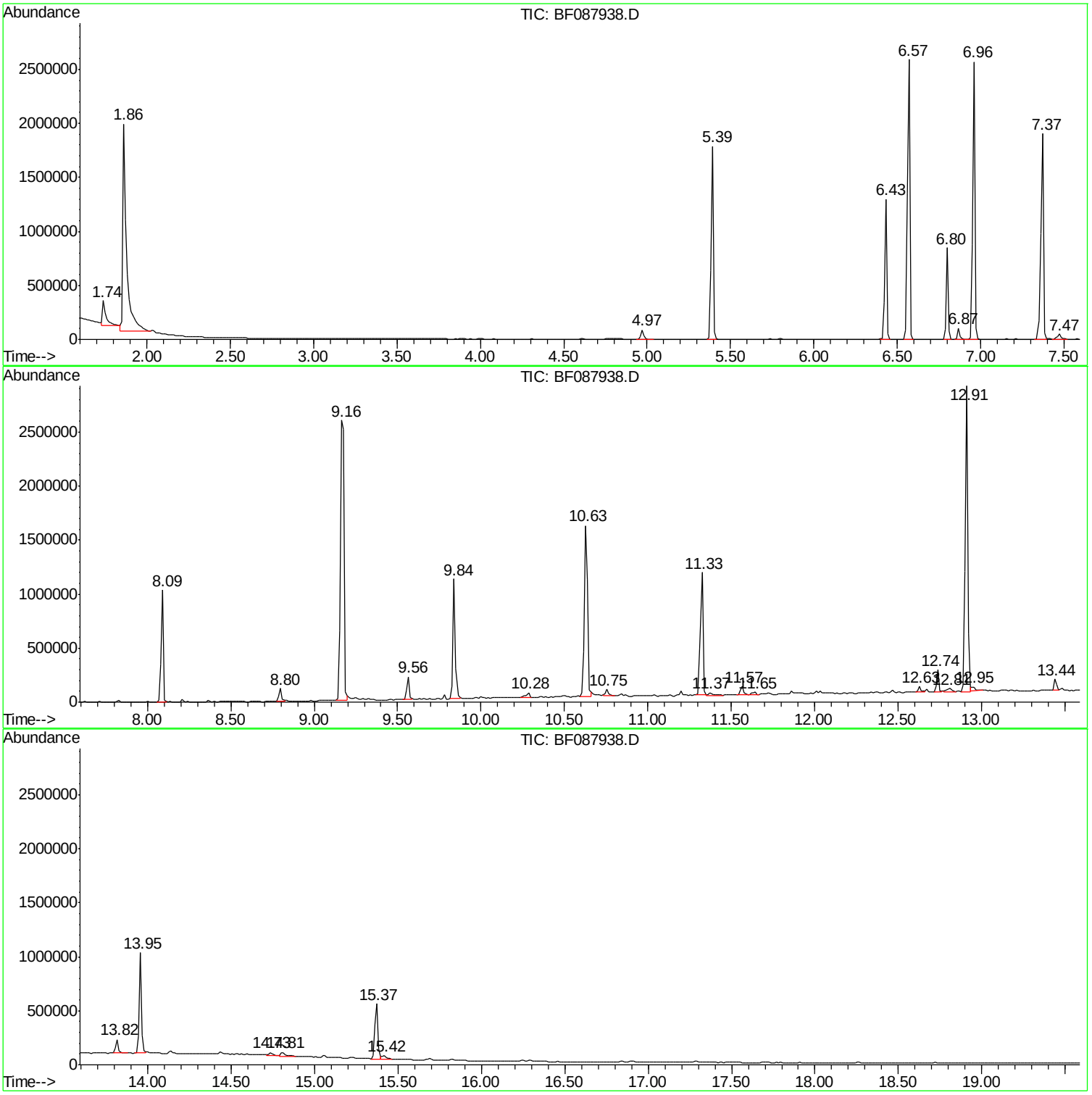
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061116\
Data File : BF087938.D
Acq On : 12 Jun 2016 9:45
Operator : UM/SJ
Sample : H3504-06
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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\BF061116\
Data File : BF087938.D
Acq On : 12 Jun 2016 9:45
Operator : UM/SJ
Sample : H3504-06
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-6

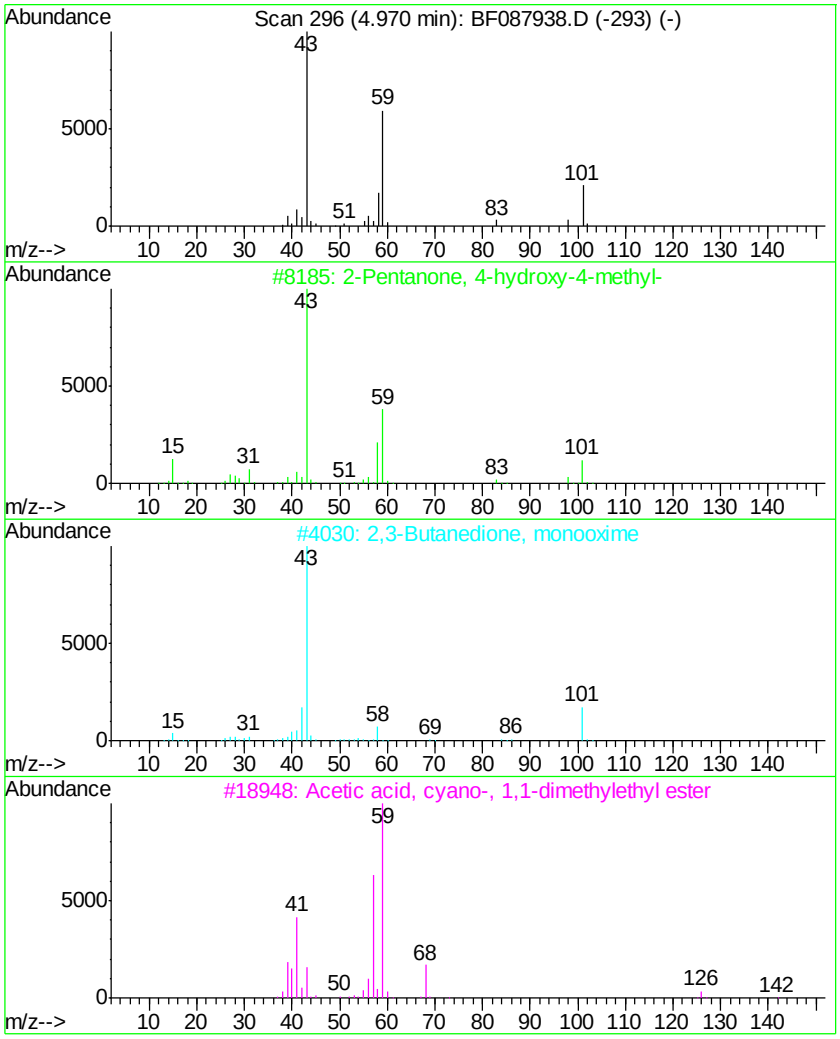
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

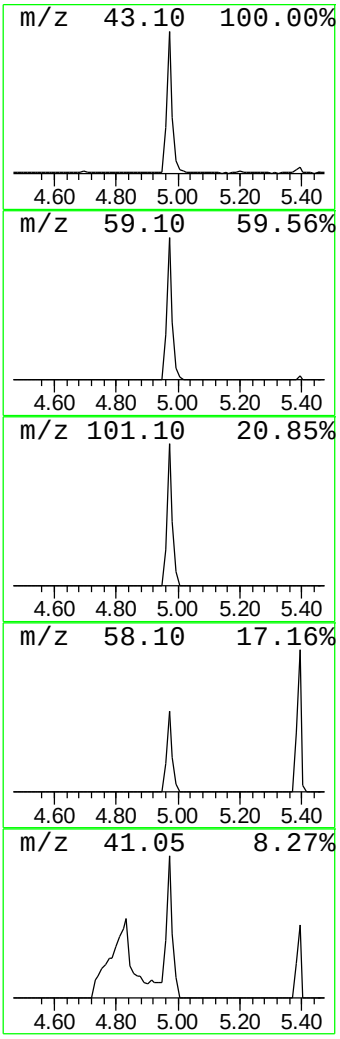
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	3.11 ng	108559	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061116\
Data File : BF087938.D
Acq On : 12 Jun 2016 9:45
Operator : UM/SJ
Sample : H3504-06
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

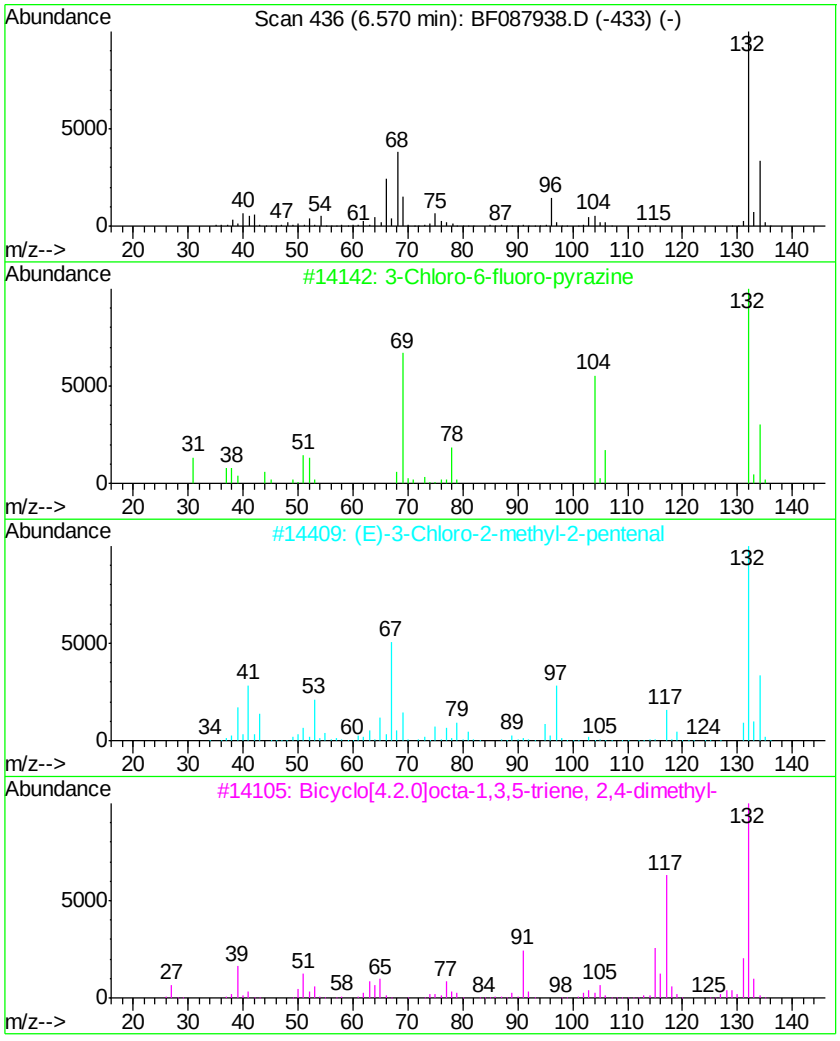
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

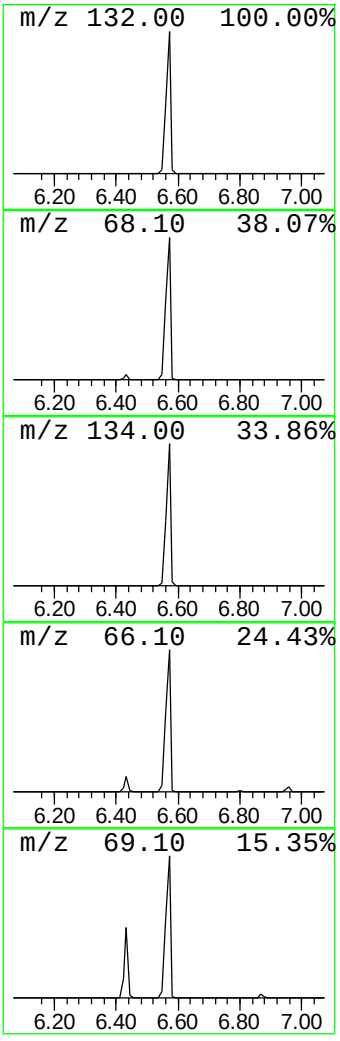
****

Peak Number 4 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	80.13 ng	2797190	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061116\
Data File : BF087938.D
Acq On : 12 Jun 2016 9:45
Operator : UM/SJ
Sample : H3504-06
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

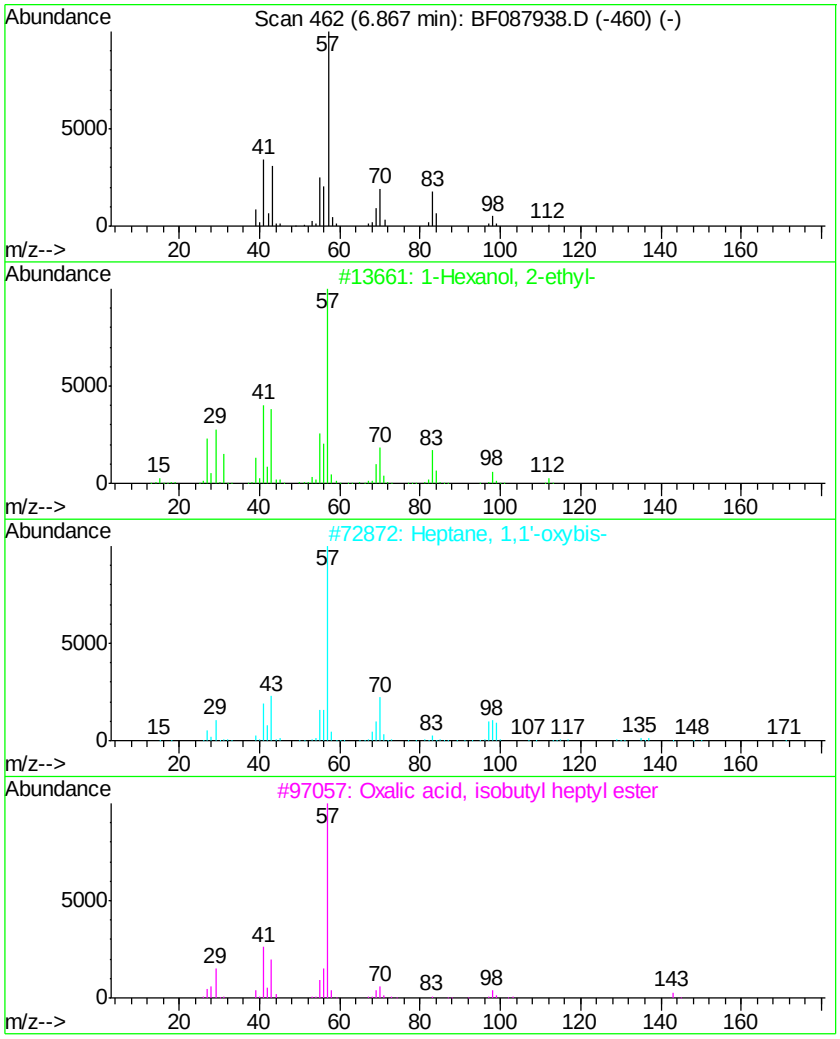
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

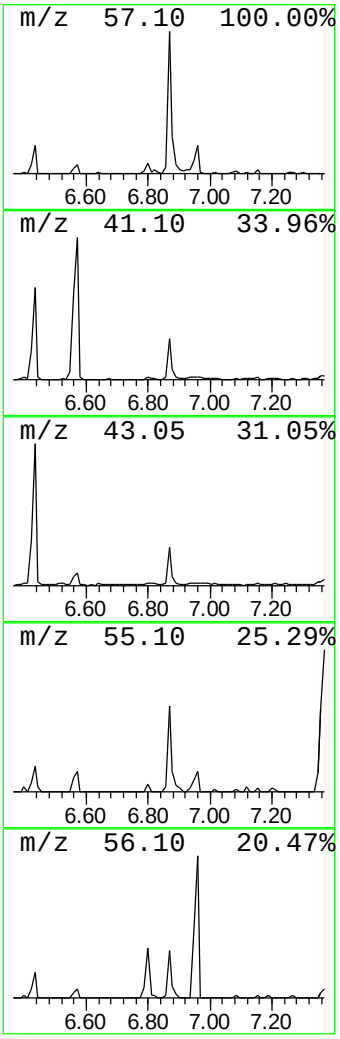
****

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.87	2.80 ng	97784	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
3	Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	47
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
5	Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	47





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061116\
Data File : BF087938.D
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Operator : UM/SJ
Sample : H3504-06
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

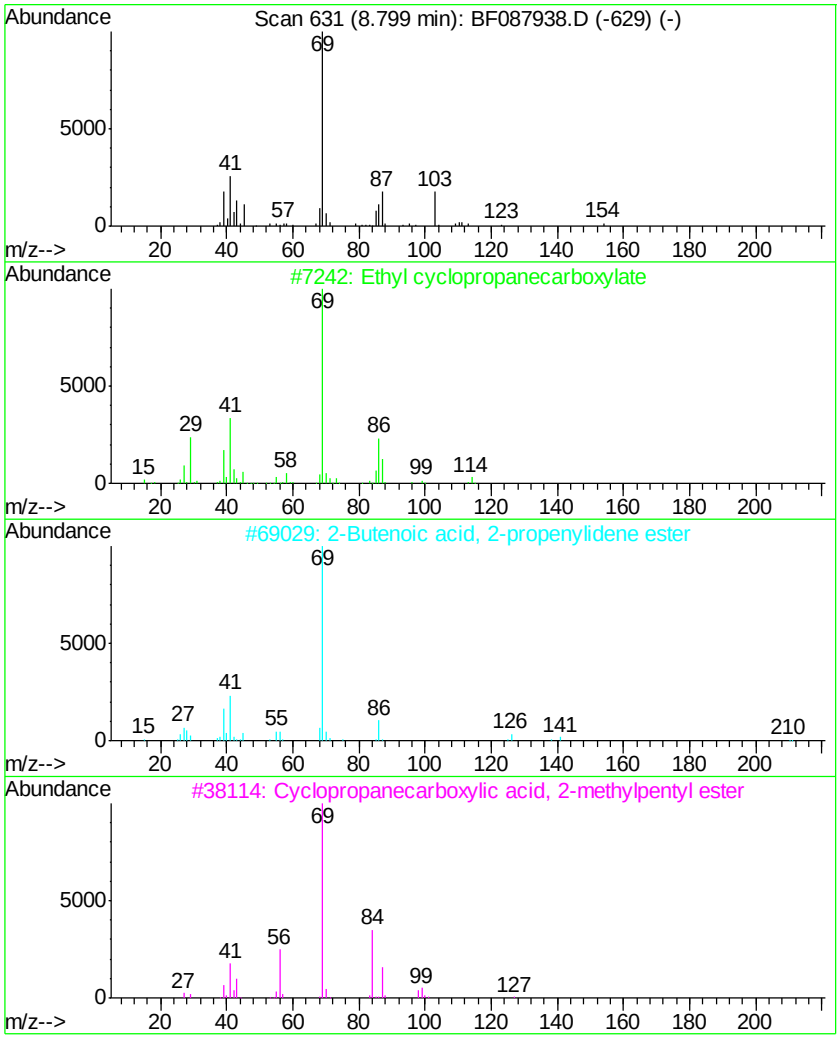
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

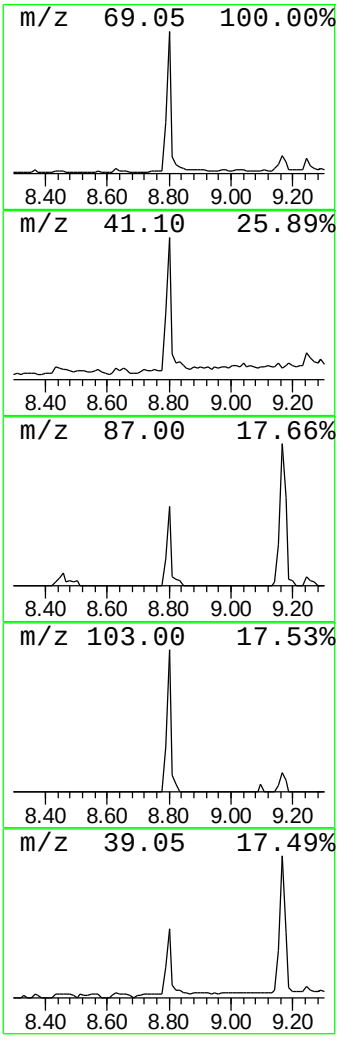
****

Peak Number 7 unknown8.80 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.80	2.74 ng	133571	Naphthalene-d8	8.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	38
2	2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	33
3	Cyclopropanecarboxylic acid, 2-m...	170	C10H18O2	1000354-65-8	33
4	Oxazole	69	C3H3NO	000288-42-6	9
5	Cyclopropanecarboxylic acid, 3-m...	154	C9H14O2	1000299-37-4	9





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Acq On : 12 Jun 2016 9:45
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Sample : H3504-06
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

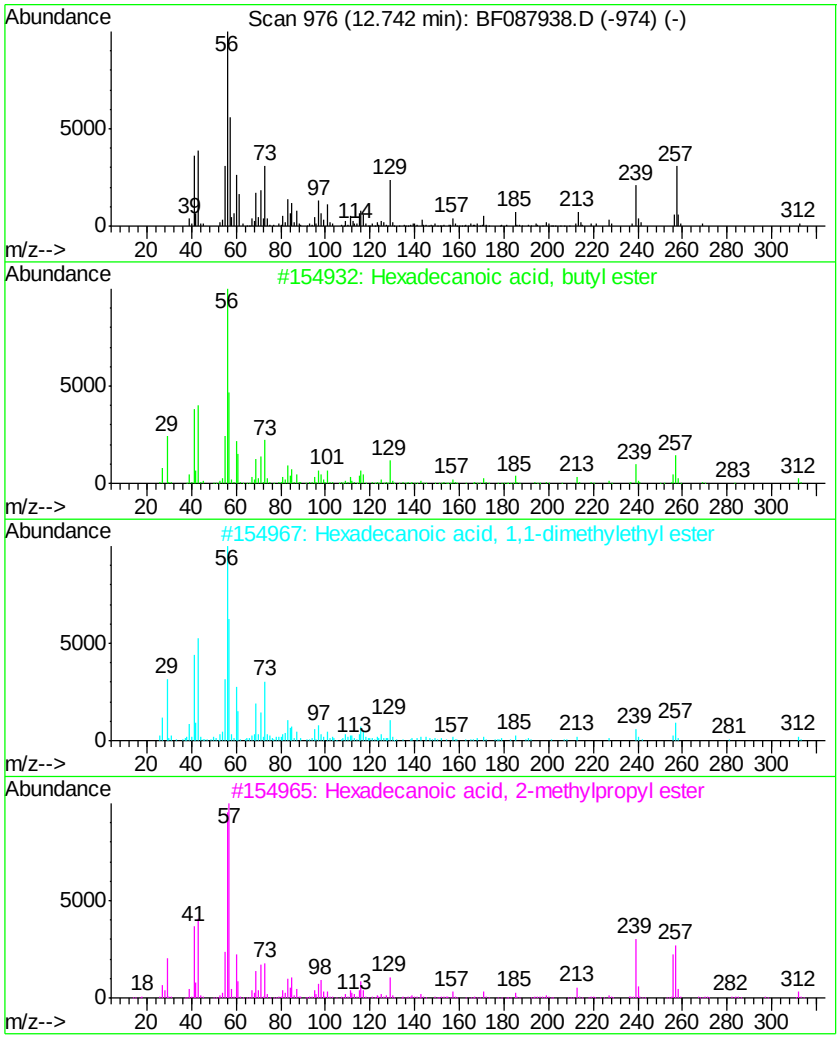
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

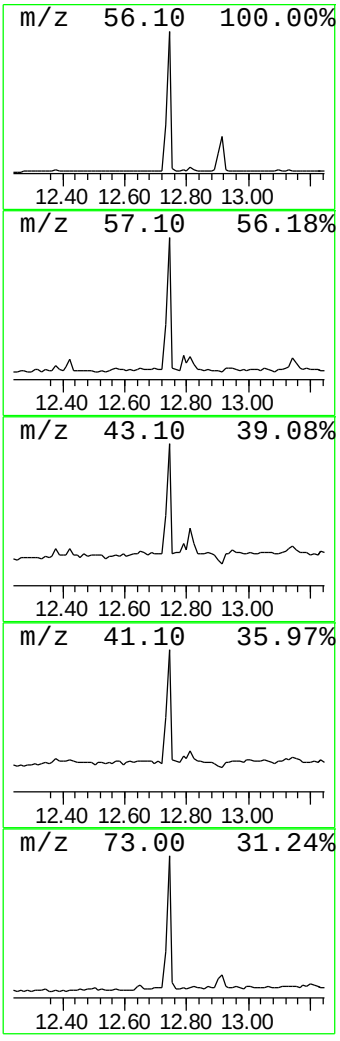
****

Peak Number 8 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	4.23 ng	187343	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	70
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	58
4	Nipecotic acid	129	C6H11NO2	000498-95-3	47
5	2,2-Dimethyl-1,3-butanediol	118	C6H14O2	000076-35-7	35





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Acq On : 12 Jun 2016 9:45
Operator : UM/SJ
Sample : H3504-06
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

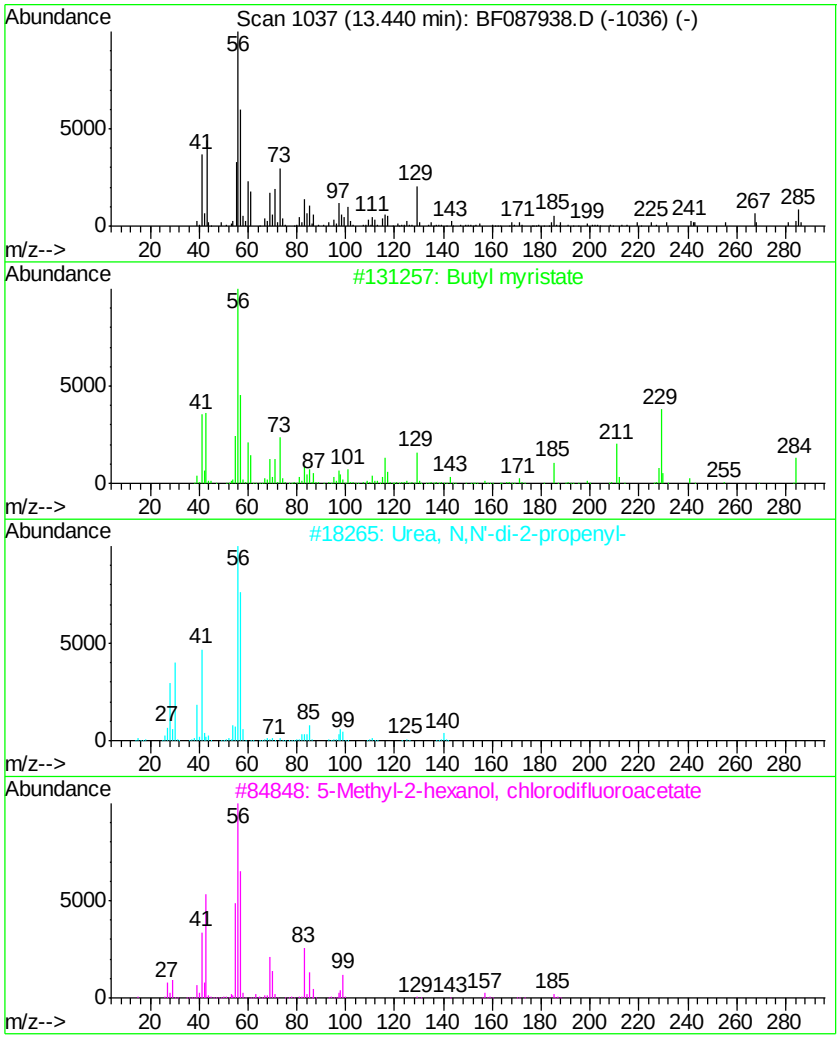
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

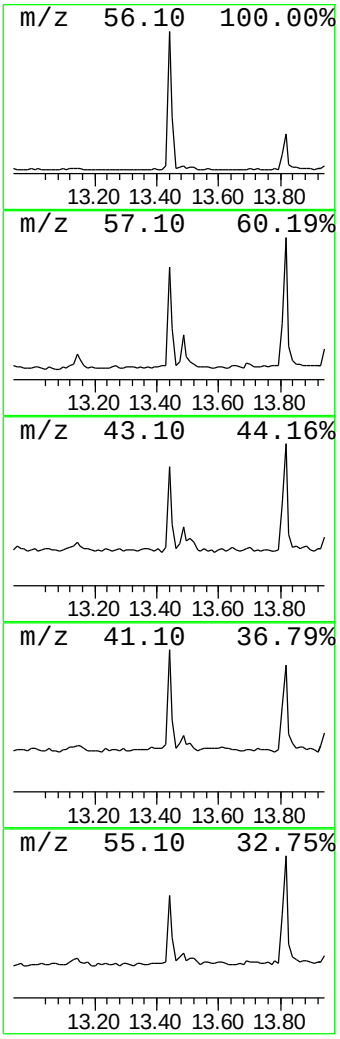
****

Peak Number 9 Butyl myristate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.44	2.56 ng	113428	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	90
2	Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	38
3	5-Methyl-2-hexanol, chlorodifluo...	228	C9H15ClF2O2	1000376-27-1	38
4	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35
5	Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	32





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Acq On : 12 Jun 2016 9:45
Operator : UM/SJ
Sample : H3504-06
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

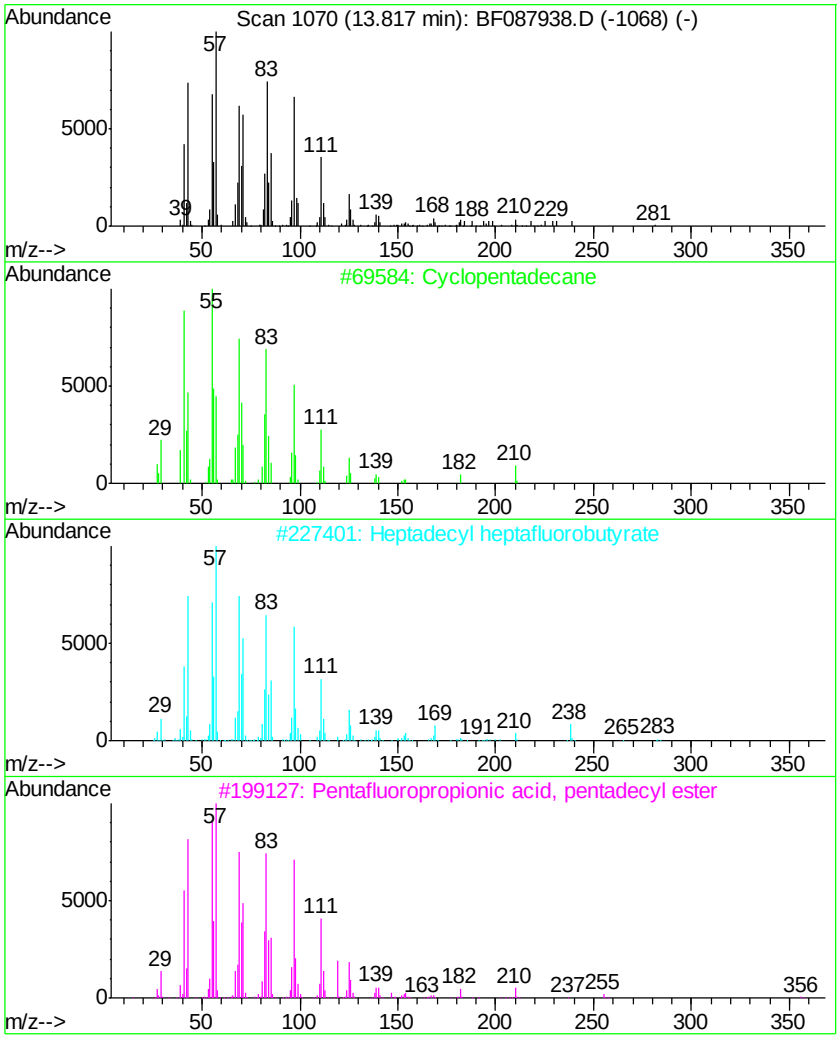
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

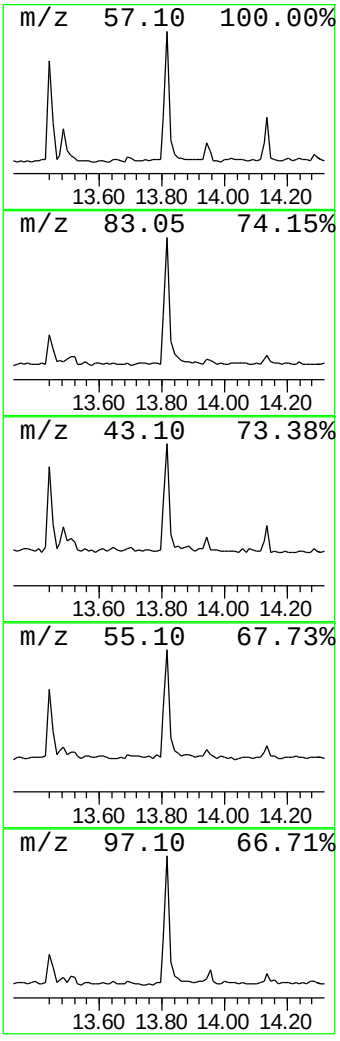
****

Peak Number 10 Cyclopentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	3.34 ng	147956	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	96
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061116\
Data File : BF087938.D
Acq On : 12 Jun 2016 9:45
Operator : UM/SJ
Sample : H3504-06
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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...	4.97	3.1	ng	108559	1	6.80	698135	20.0
unknown6.57	6.57	80.1	ng	2797190	1	6.80	698135	20.0
1-Hexanol, 2-ethyl-	6.87	2.8	ng	97784	1	6.80	698135	20.0
unknown8.80	8.80	2.7	ng	133571	2	8.09	976055	20.0
Hexadecanoic acid...	12.74	4.2	ng	187343	5	13.95	885677	20.0
Butyl myristate	13.44	2.6	ng	113428	5	13.95	885677	20.0
Cyclopentadecane	13.82	3.3	ng	147956	5	13.95	885677	20.0