LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042016\
Data File : BF086338.D
Acq On : 21 Apr 2016 5:18
Operator : UM/SJ
Sample : H2569-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LCF-SW1

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-BF042016.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	2.133	3	4	32	rVB	225089	808837	19.09%	2.131%
2	5.059	258	260	265	rBV	236284	322027	7.60%	0.848%
3	5.470	293	296	298	rBV	3888928	4097660	96.73%	10.795%
4	5.962	336	339	346	rVB2	12948	44211	1.04%	0.116%
5	6.499	383	386	389	rBV	3113428	3901349	92.10%	10.278%
6	6.636	395	398	400	rBV	4163611	4236183	100.00%	11.160%
7	6.865	416	418	429	rVB	1240061	1298947	30.66%	3.422%
8	7.025	429	432	434	rBV	3386903	3314510	78.24%	8.732%
9	7.425	465	467	470	rBV	1583394	2431886	57.41%	6.406%
10	7.527	474	476	483	rVB	105737	164111	3.87%	0.432%
11	8.156	528	531	533	rBV	1212569	1443549	34.08%	3.803%
12	9.231	622	625	627	rBV	3900954	3723562	87.90%	9.809%
13	9.311	631	632	638	rVB	48748	72169	1.70%	0.190%
14	9.619	657	659	661	rBV	629553	608875	14.37%	1.604%
15	9.836	676	678	680	rBV	74184	94704	2.24%	0.249%
16	9.905	682	684	687	rVV	1387387	1283184	30.29%	3.380%
17	10.339	721	722	724	rVB	197295	152662	3.60%	0.402%
18	10.556	738	741	745	rBV	61603	110348	2.60%	0.291%
19	10.694	750	753	759	rVV	1715642	1968468	46.47%	5.186%
20	10.808	762	763	770	rVB	150812	257263	6.07%	0.678%
21	11.265	801	803	804	rBV	94749	108685	2.57%	0.286%
22	11.391	812	814	817	rBV	1137824	1175274	27.74%	3.096%
23	11.688	838	840	842	rVB	73759	65803	1.55%	0.173%
24	12.854	939	942	943	rBV	65613	61028	1.44%	0.161%
25	12.979	950	953	955	rBV	2257282	2991942	70.63%	7.882%
26	13.208	971	973	978	rBV	83307	86774	2.05%	0.229%
27	13.551	1001	1003	1005	rBV	163322	153159	3.62%	0.403%
28	13.882	1030	1032	1033	rBV	182711	210996	4.98%	0.556%
29	13.905	1033	1034	1039	rVV	102700	200895	4.74%	0.529%
30	14.020	1042	1044	1051	rVV	810637	1155995	27.29%	3.045%
31	14.134	1051	1054	1056	rVV3	28364	43148	1.02%	0.114%
32	14.191	1057	1059	1062	rBV	173749	203174	4.80%	0.535%
33	14.500	1083	1086	1088	rBV	178453	189906	4.48%	0.500%
34	14.797	1108	1112	1115	rBV2	101543	154997	3.66%	0.408%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042016\
Data File : BF086338.D
Acq On : 21 Apr 2016 5:18
Operator : UM/SJ
Sample : H2569-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LCF-SW1

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-BF042016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.865	1116	1118	1121	rBV	42839	64349	1.52%	0.170%
36	15.460	1167	1170	1176	rBV	458763	759062	17.92%	2.000%

Sum of corrected areas: 37959692

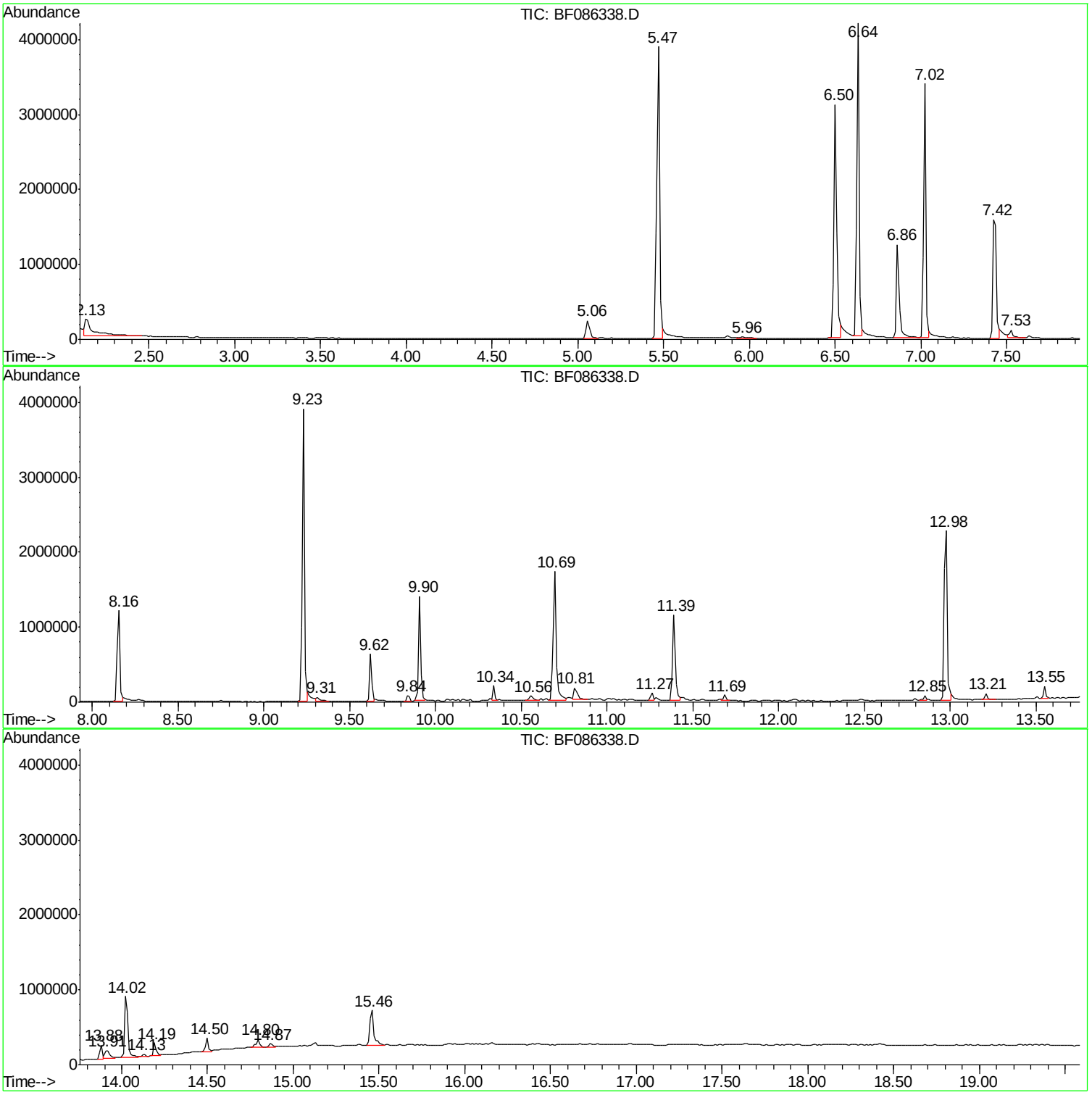
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042016\
Data File : BF086338.D
Acq On : 21 Apr 2016 5:18
Operator : UM/SJ
Sample : H2569-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LCF-SW1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042016\
Data File : BF086338.D
Acq On : 21 Apr 2016 5:18
Operator : UM/SJ
Sample : H2569-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LCF-SW1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

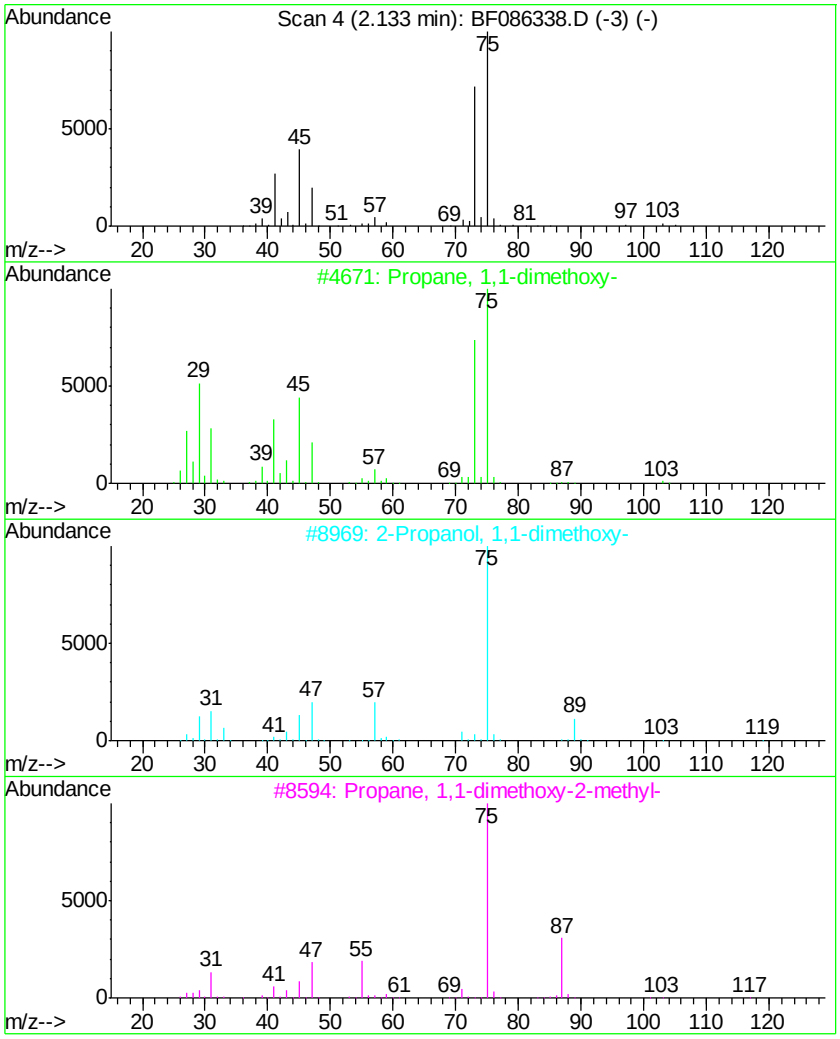
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

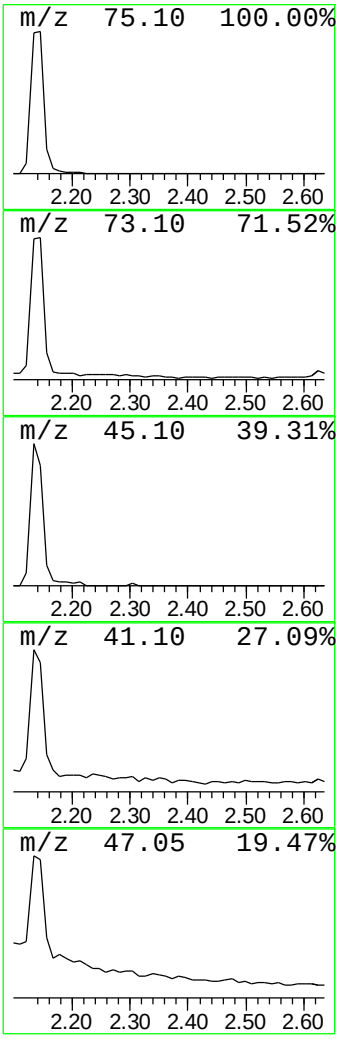
****

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	12.45 ng	808837	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2	2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	42
3	Propane, 1,1-dimethoxy-2-methyl-	118	C6H14O2	041632-89-7	33
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042016\
Data File : BF086338.D
Acq On : 21 Apr 2016 5:18
Operator : UM/SJ
Sample : H2569-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LCF-SW1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

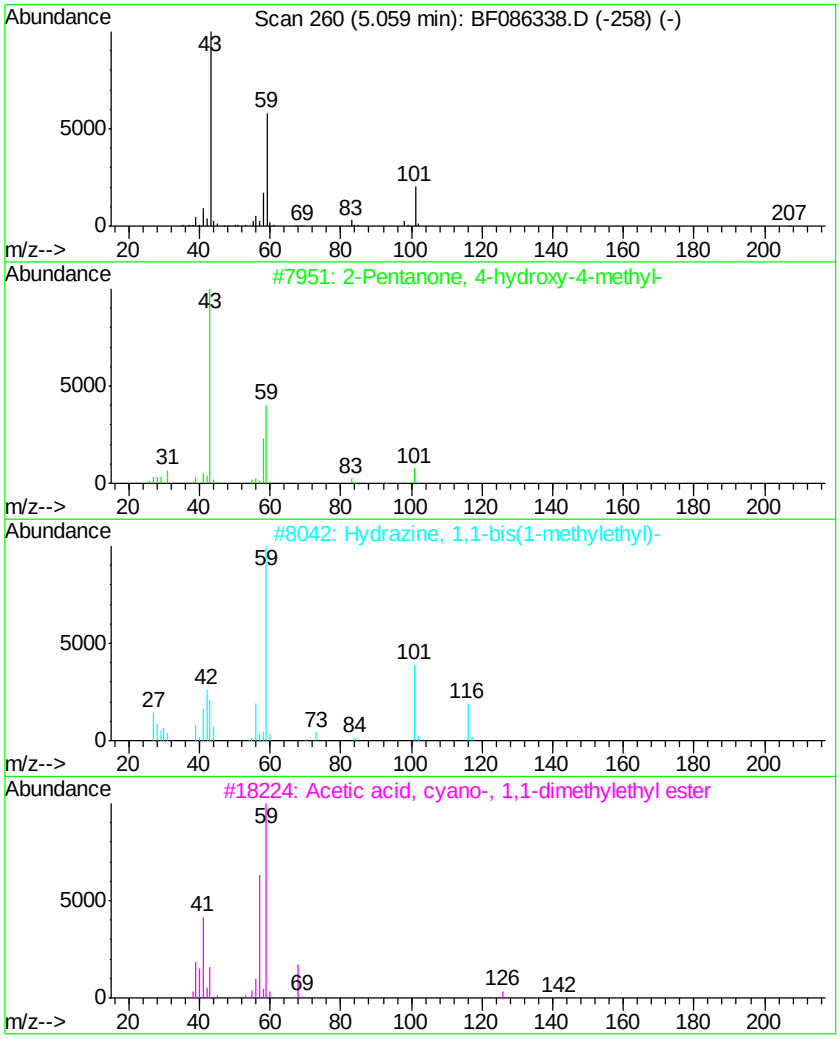
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

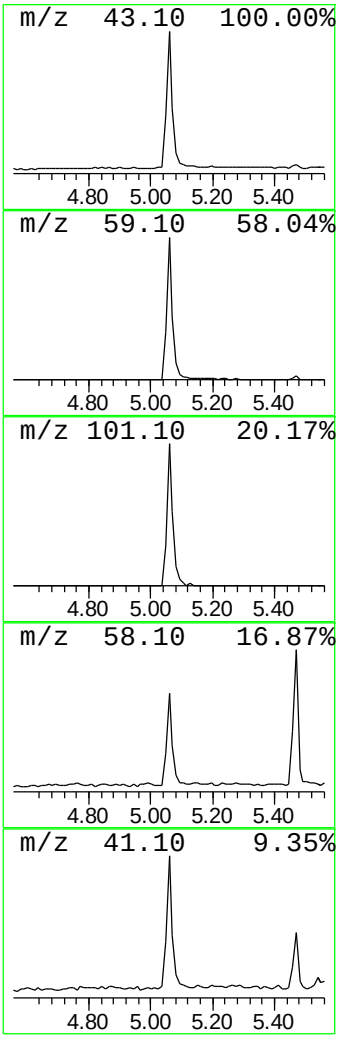
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	4.96 ng	322027	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
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\BF042016\
Data File : BF086338.D
Acq On : 21 Apr 2016 5:18
Operator : UM/SJ
Sample : H2569-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LCF-SW1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

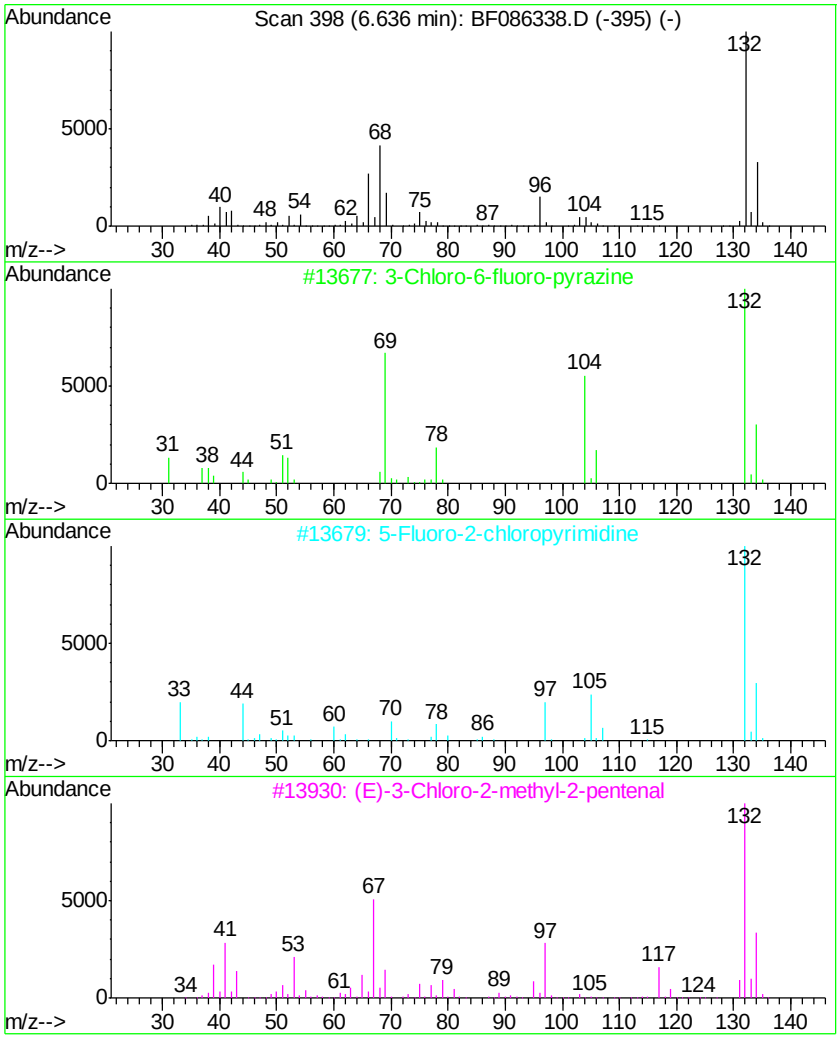
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

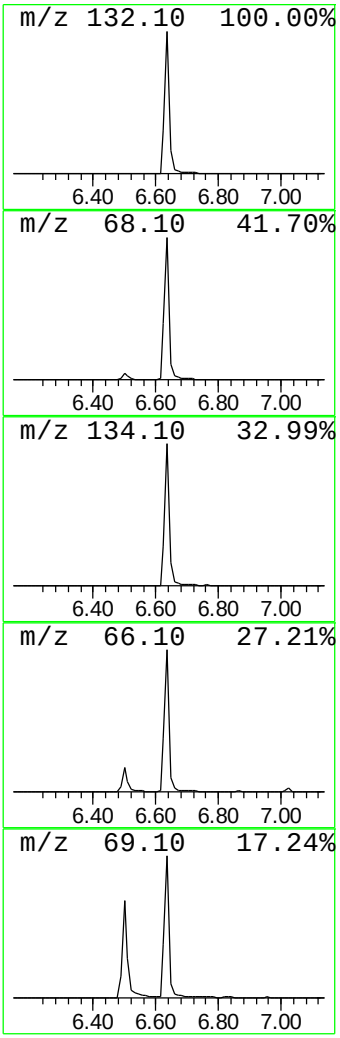
****

Peak Number 3 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	65.22 ng	4236180	1,4-Dichlorobenzene-d4	6.86

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	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042016\
Data File : BF086338.D
Acq On : 21 Apr 2016 5:18
Operator : UM/SJ
Sample : H2569-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LCF-SW1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

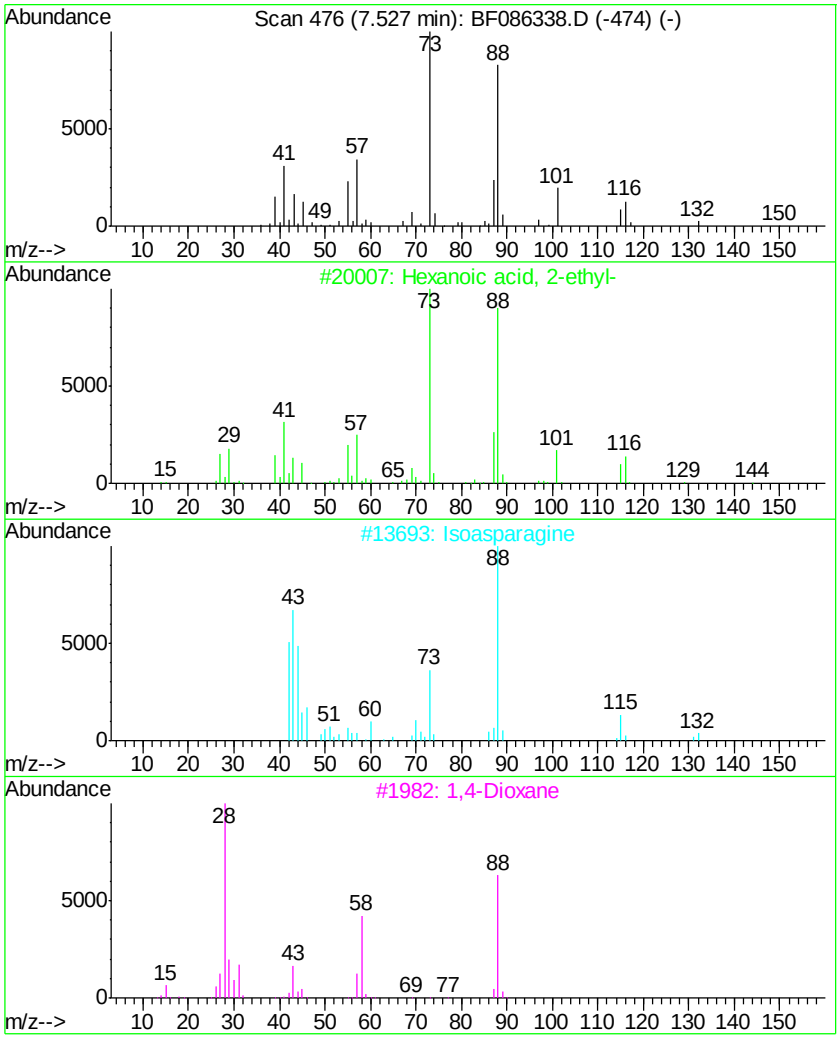
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

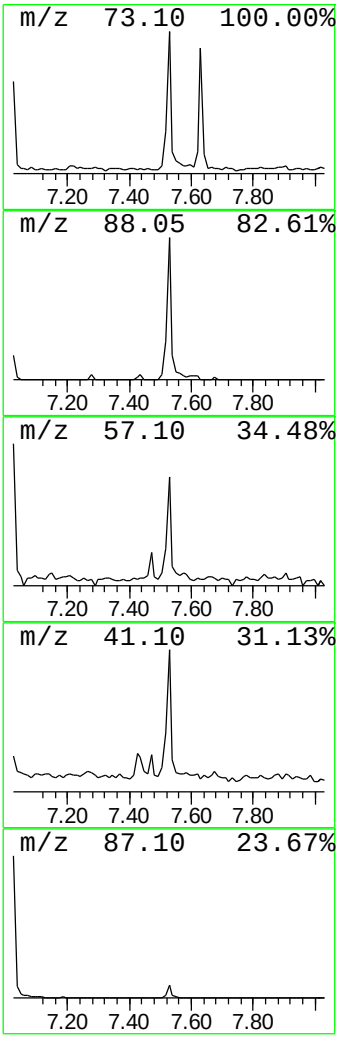
****

Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.53	2.27 ng	164111	Naphthalene-d8	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Isoasparagine	132	C4H8N2O3	1000130-17-5	42
3	1,4-Dioxane	88	C4H8O2	000123-91-1	37
4	Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	36
5	Hydroxypivalic acid	118	C5H10O3	004835-90-9	36





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042016\
Data File : BF086338.D
Acq On : 21 Apr 2016 5:18
Operator : UM/SJ
Sample : H2569-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LCF-SW1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

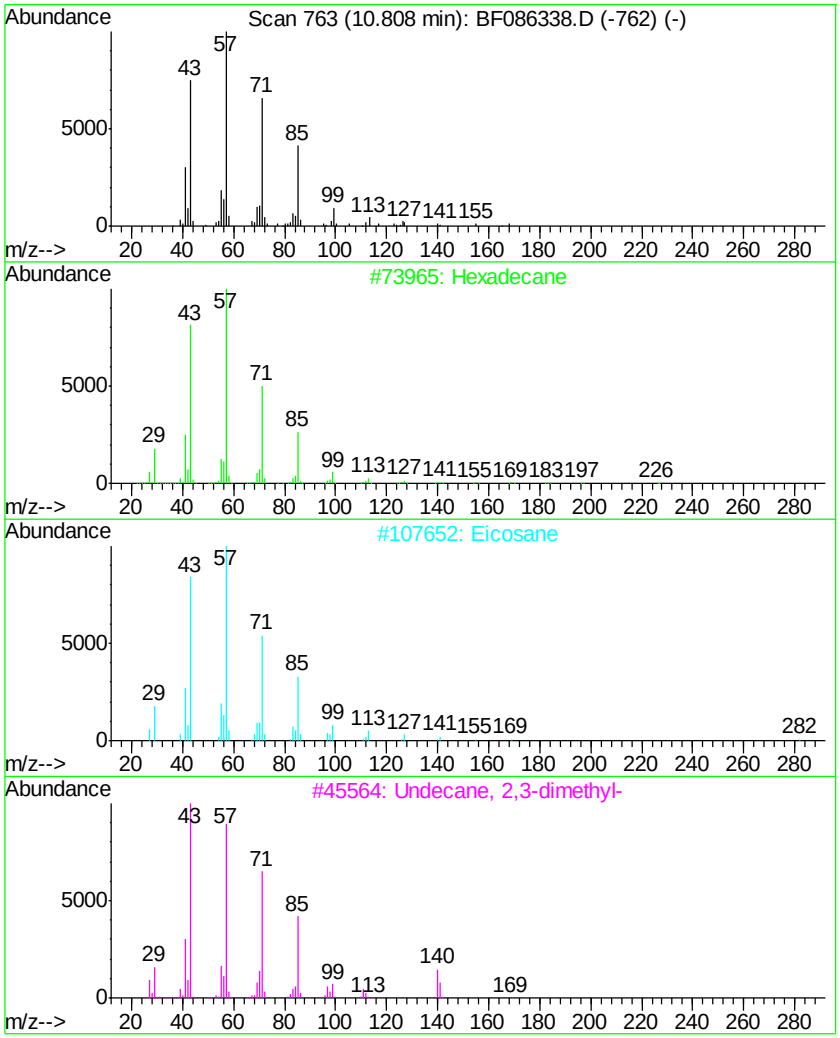
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

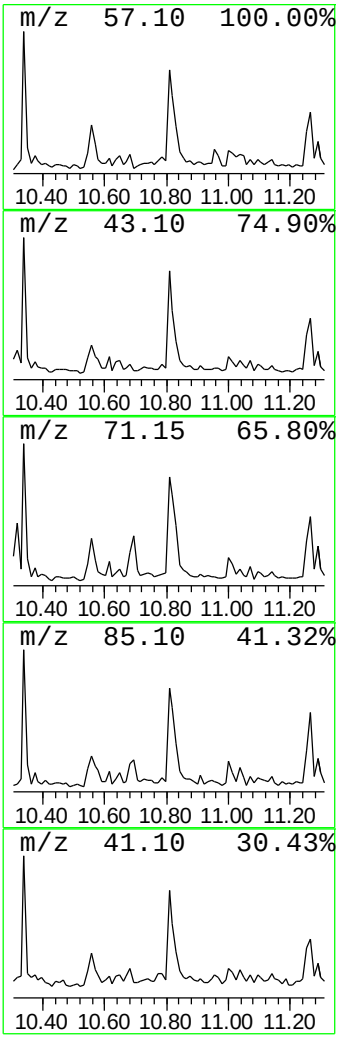
****

Peak Number 7 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.81	4.38 ng	257263	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	80
2	Eicosane	282	C20H42	000112-95-8	80
3	Undecane, 2,3-dimethyl-	184	C13H28	017312-77-5	72
4	Nonane, 5-butyl-	184	C13H28	017312-63-9	59
5	Tridecane, 2-methyl-	198	C14H30	001560-96-9	53





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Data File : BF086338.D
Acq On : 21 Apr 2016 5:18
Operator : UM/SJ
Sample : H2569-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LCF-SW1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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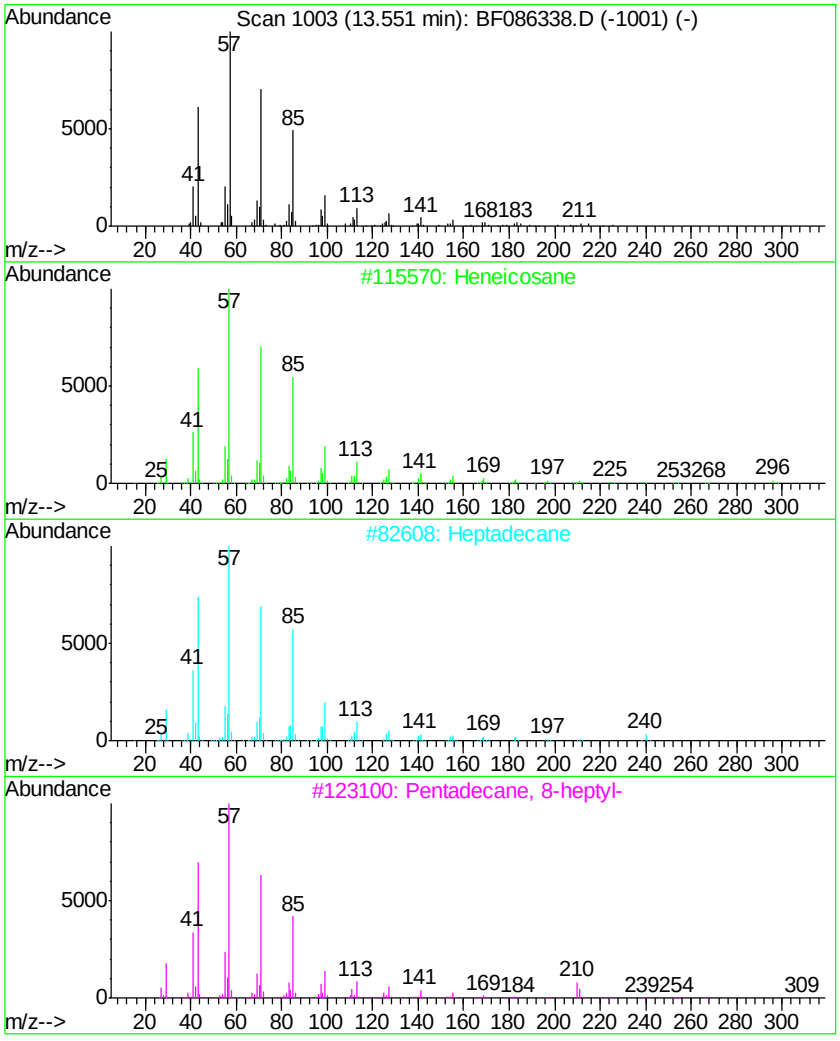
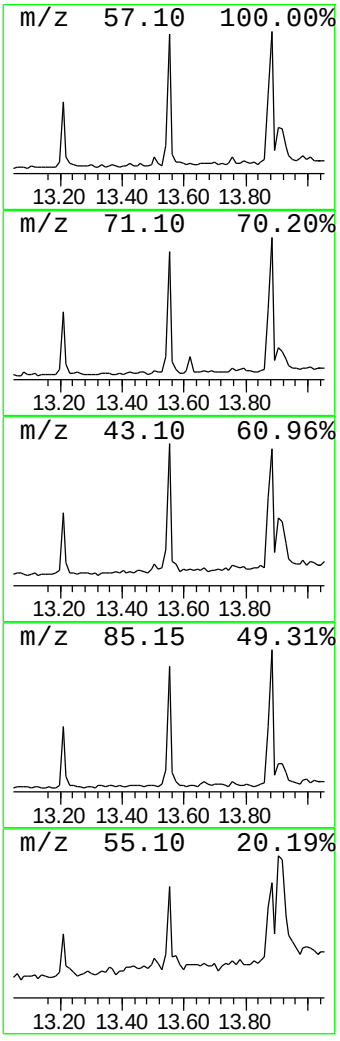
Peak Number 8 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	2.65 ng	153159	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
4	Tetracosane	338	C24H50	000646-31-1	90
5	Triacontane	422	C30H62	000638-68-6	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042016\
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Operator : UM/SJ
Sample : H2569-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LCF-SW1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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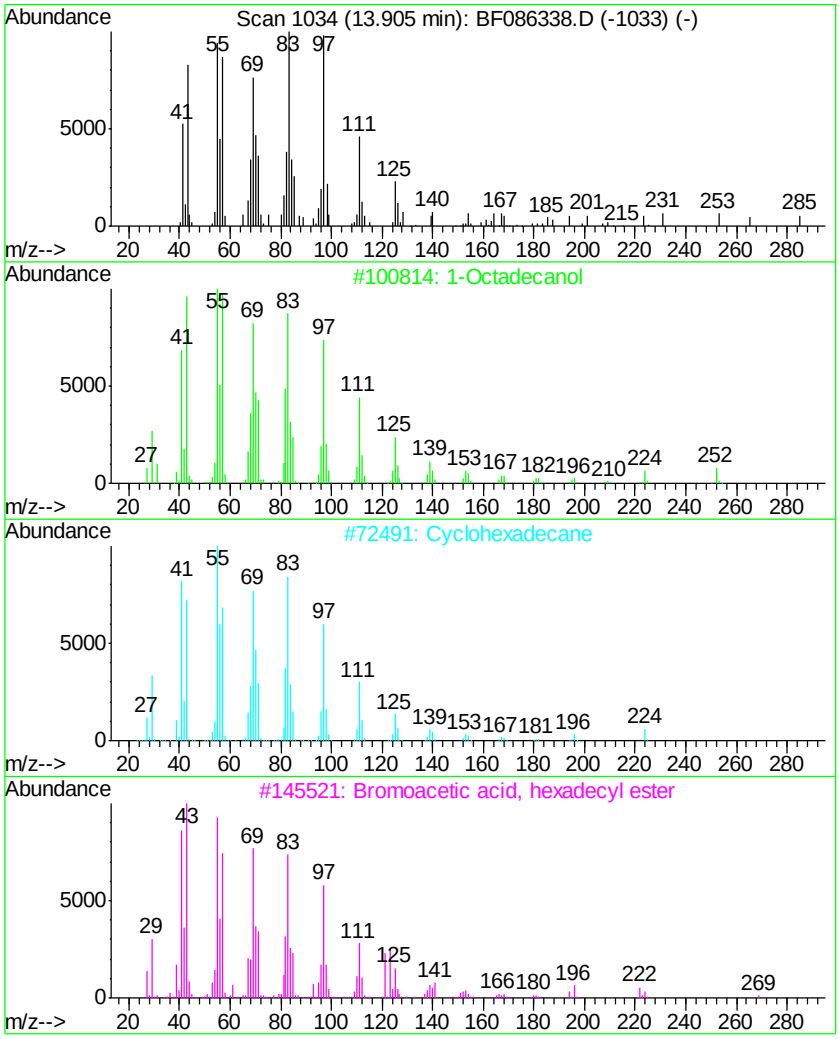
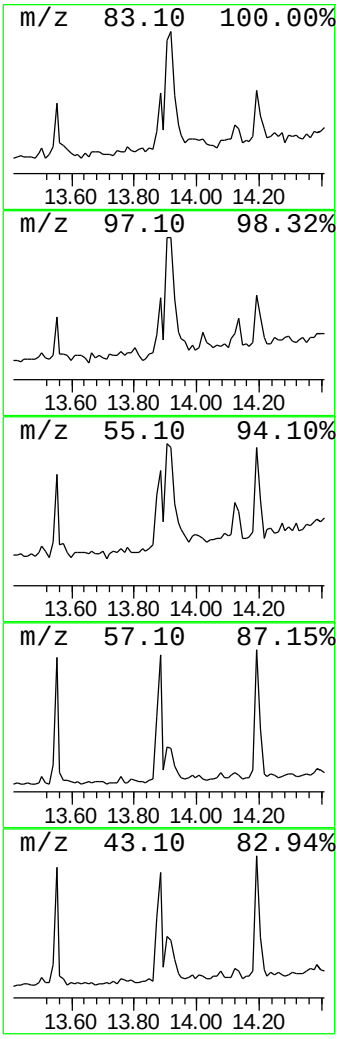
Peak Number 10 1-Octadecanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.91	3.48 ng	200895	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanol	270	C18H38O	000112-92-5	93
2	Cyclohexadecane	224	C16H32	000295-65-8	91
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	87
4	1-Hexadecanol	242	C16H34O	036653-82-4	87
5	Chloroacetic acid, pentadecyl ester	304	C17H33ClO2	070301-47-2	87





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Acq On : 21 Apr 2016 5:18
Operator : UM/SJ
Sample : H2569-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LCF-SW1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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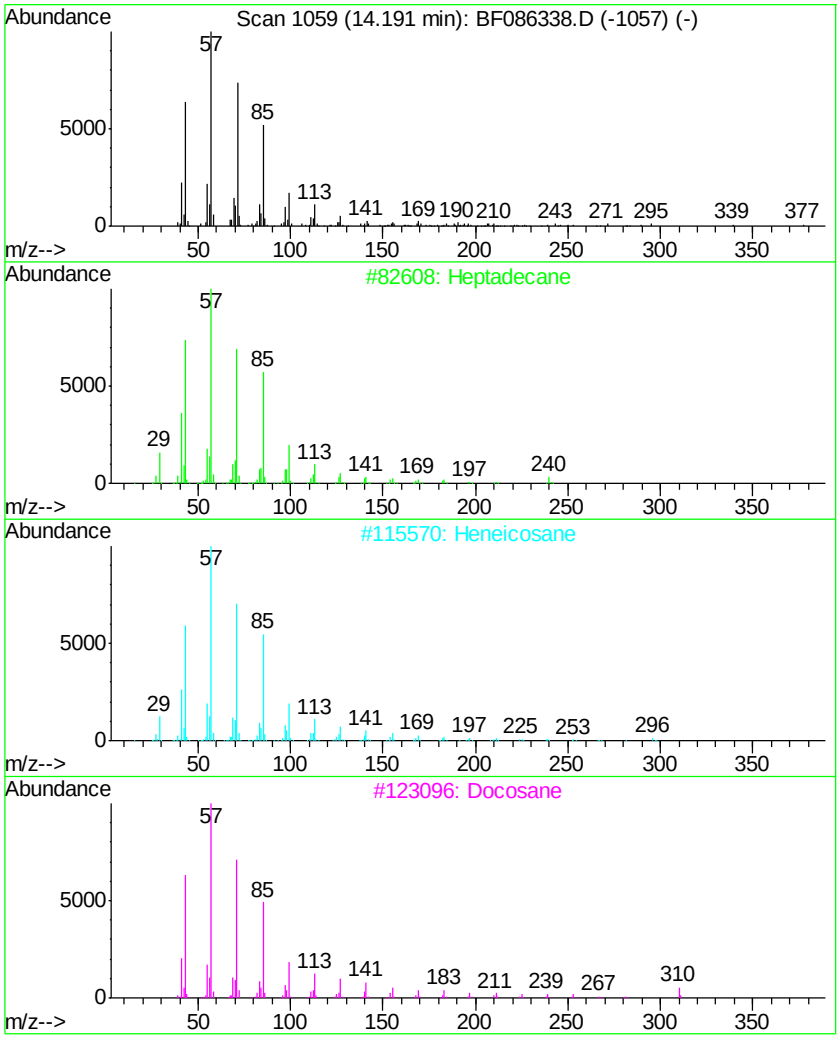
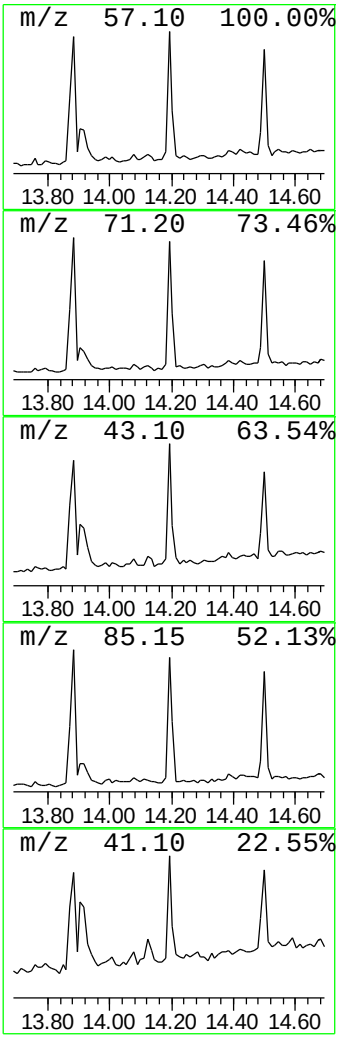
Peak Number 11 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.19	3.52 ng	203174	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Docosane	310	C22H46	000629-97-0	90
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042016\
Data File : BF086338.D
Acq On : 21 Apr 2016 5:18
Operator : UM/SJ
Sample : H2569-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LCF-SW1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

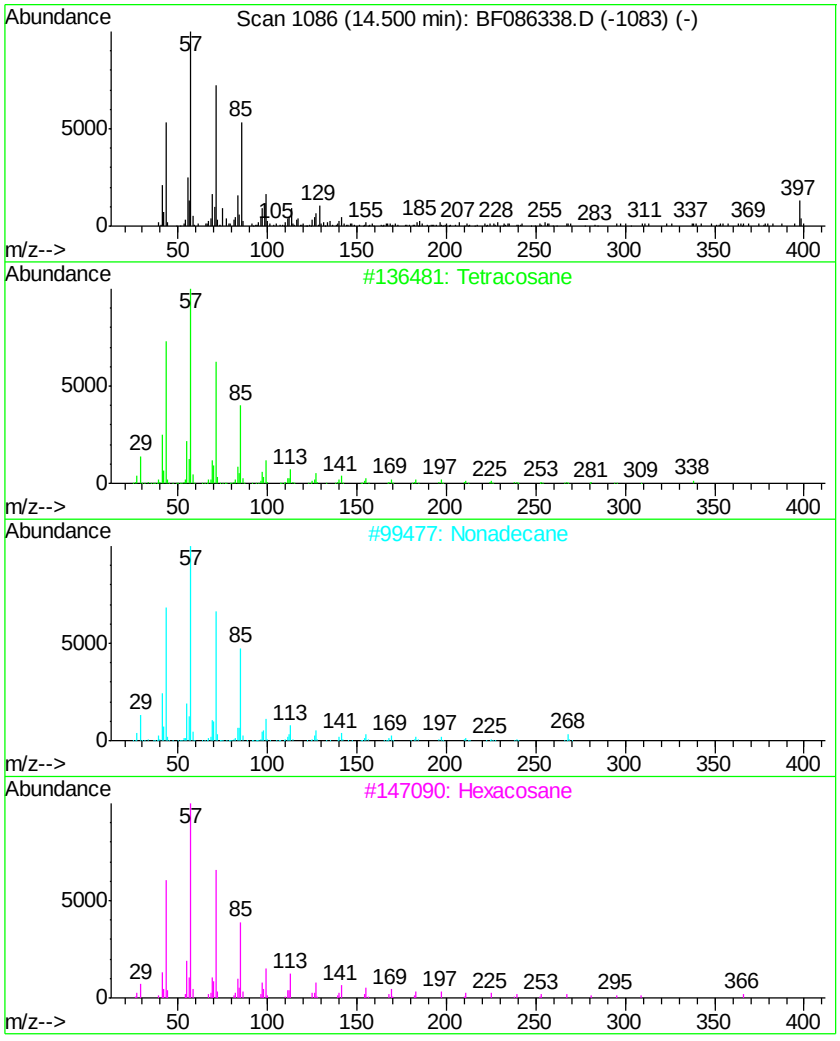
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

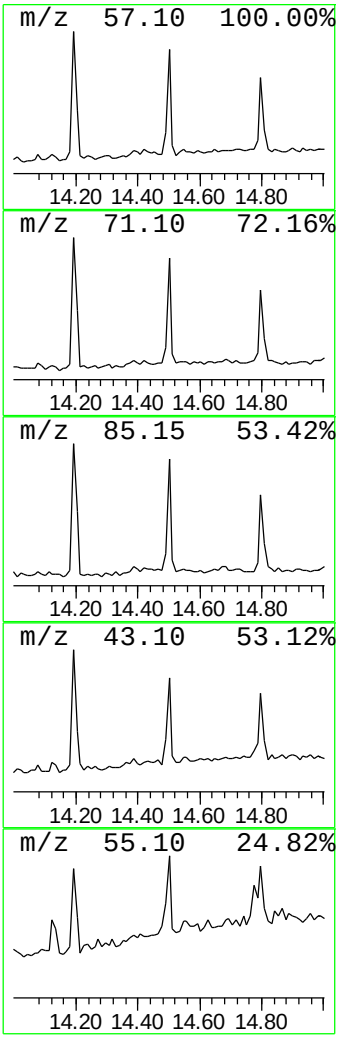
****

Peak Number 12 Tetracosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	3.29 ng	189906	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	96
2	Nonadecane	268	C19H40	000629-92-5	93
3	Hexacosane	366	C26H54	000630-01-3	83
4	Hexadecane	226	C16H34	000544-76-3	70
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	68





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Data File : BF086338.D
Acq On : 21 Apr 2016 5:18
Operator : UM/SJ
Sample : H2569-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LCF-SW1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

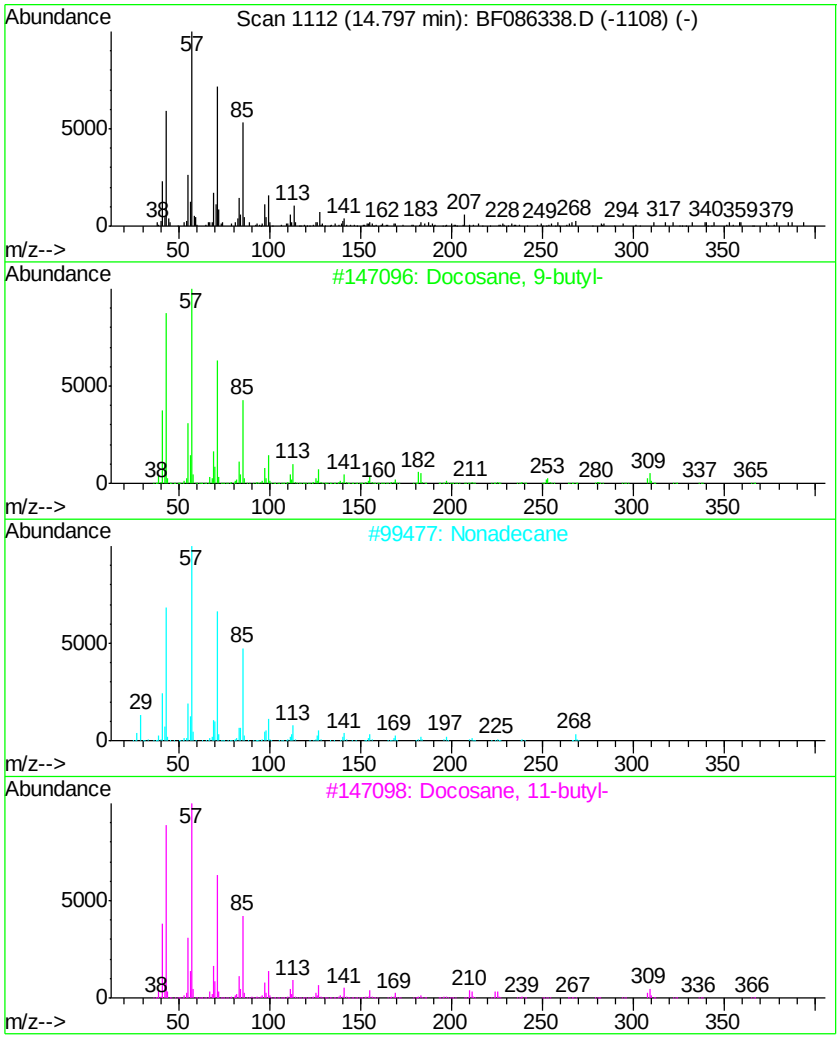
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

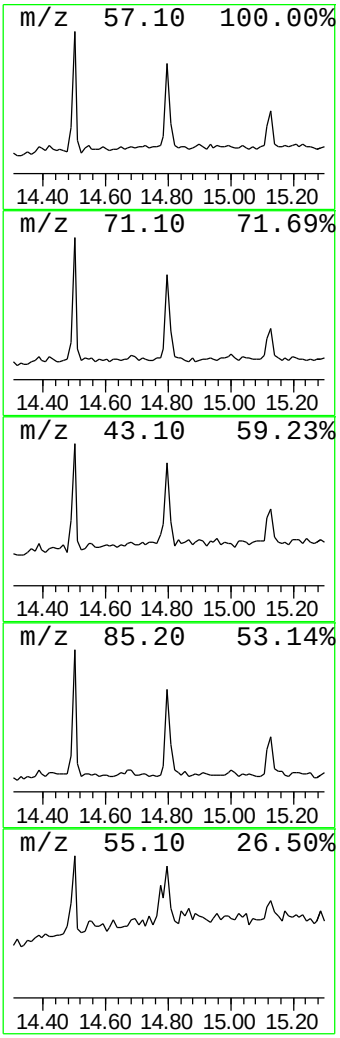
****

Peak Number 13 Docosane, 9-butyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	4.08 ng	154997	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 9-butyl-	366	C26H54	055282-14-9	93
2	Nonadecane	268	C19H40	000629-92-5	91
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	90
4	Tetracosane	338	C24H50	000646-31-1	87
5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042016\
Data File : BF086338.D
Acq On : 21 Apr 2016 5:18
Operator : UM/SJ
Sample : H2569-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LCF-SW1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 1,1-dime...	2.13	12.4	ng	808837	1	6.86	1298950	20.0
2-Pentanone, 4-hy...	5.06	5.0	ng	322027	1	6.86	1298950	20.0
unknown6.64	6.64	65.2	ng	4236180	1	6.86	1298950	20.0
Hexanoic acid, 2-...	7.53	2.3	ng	164111	2	8.16	1443550	20.0
Hexadecane	10.81	4.4	ng	257263	4	11.39	1175270	20.0
Heneicosane	13.55	2.6	ng	153159	5	14.02	1156000	20.0
1-Octadecanol	13.91	3.5	ng	200895	5	14.02	1156000	20.0
Heptadecane	14.19	3.5	ng	203174	5	14.02	1156000	20.0
Tetracosane	14.50	3.3	ng	189906	5	14.02	1156000	20.0
Docosane, 9-butyl-	14.80	4.1	ng	154997	6	15.46	759062	20.0