LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051316\
Data File : BF086986.D
Acq On : 13 May 2016 22:50
Operator : UM/SJ
Sample : H2877-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-35

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-BF050916.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	1.735	12	13	30	rVB	3389829	5867299	100.00%	13.713%
2	4.742	275	276	284	rBV	48220	96060	1.64%	0.225%
3	5.199	314	316	328	rBV	1577257	2007793	34.22%	4.693%
4	6.273	407	410	417	rBV	1014102	1320766	22.51%	3.087%
5	6.376	417	419	422	rBV	2608963	3502160	59.69%	8.185%
6	6.605	437	439	442	rBV	694491	901864	15.37%	2.108%
7	6.765	451	453	456	rBV	3440697	3154980	53.77%	7.374%
8	7.187	487	490	492	rBV	2980876	3214423	54.79%	7.513%
9	7.896	550	552	555	rBV	1282012	1199793	20.45%	2.804%
10	8.982	644	647	649	rBV	4758316	5075384	86.50%	11.862%
11	9.382	679	682	686	rVB2	85011	129408	2.21%	0.302%
12	9.645	702	705	708	rBV	1488850	1362131	23.22%	3.184%
13	10.091	741	744	746	rBV	96796	86047	1.47%	0.201%
14	10.434	771	774	777	rBV	2782996	3099437	52.83%	7.244%
15	10.559	783	785	790	rVB	101717	110392	1.88%	0.258%
16	11.119	832	834	837	rBV	1294700	1311419	22.35%	3.065%
17	11.611	874	877	880	rBV	49178	98379	1.68%	0.230%
18	11.679	880	883	890	rVB	479403	617025	10.52%	1.442%
19	12.377	940	944	949	rBV2	150227	359968	6.14%	0.841%
20	12.457	949	951	956	rVV	162730	207508	3.54%	0.485%
21	12.548	956	959	961	rVB	436774	494438	8.43%	1.156%
22	12.617	964	965	970	rVB	111407	113259	1.93%	0.265%
23	12.708	970	973	976	rBV	3646426	5073011	86.46%	11.857%
24	13.245	1018	1020	1022	rBV	457469	395838	6.75%	0.925%
25	13.622	1050	1053	1062	rBV	128974	213322	3.64%	0.499%
26	13.748	1062	1064	1067	rBV	1455575	1348056	22.98%	3.151%
27	13.931	1078	1080	1085	rVB	109194	105690	1.80%	0.247%
28	14.240	1103	1107	1109	rBV	86625	103496	1.76%	0.242%
29	14.525	1130	1132	1135	rBV	74135	85097	1.45%	0.199%
30	14.823	1155	1158	1161	rBV	60352	73774	1.26%	0.172%
31	15.108	1180	1183	1185	rBV	893084	995221	16.96%	2.326%
32	15.931	1252	1255	1263	rVB2	24545	62252	1.06%	0.145%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051316\
Data File : BF086986.D
Acq On : 13 May 2016 22:50
Operator : UM/SJ
Sample : H2877-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-35

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-BF050916.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 42785690

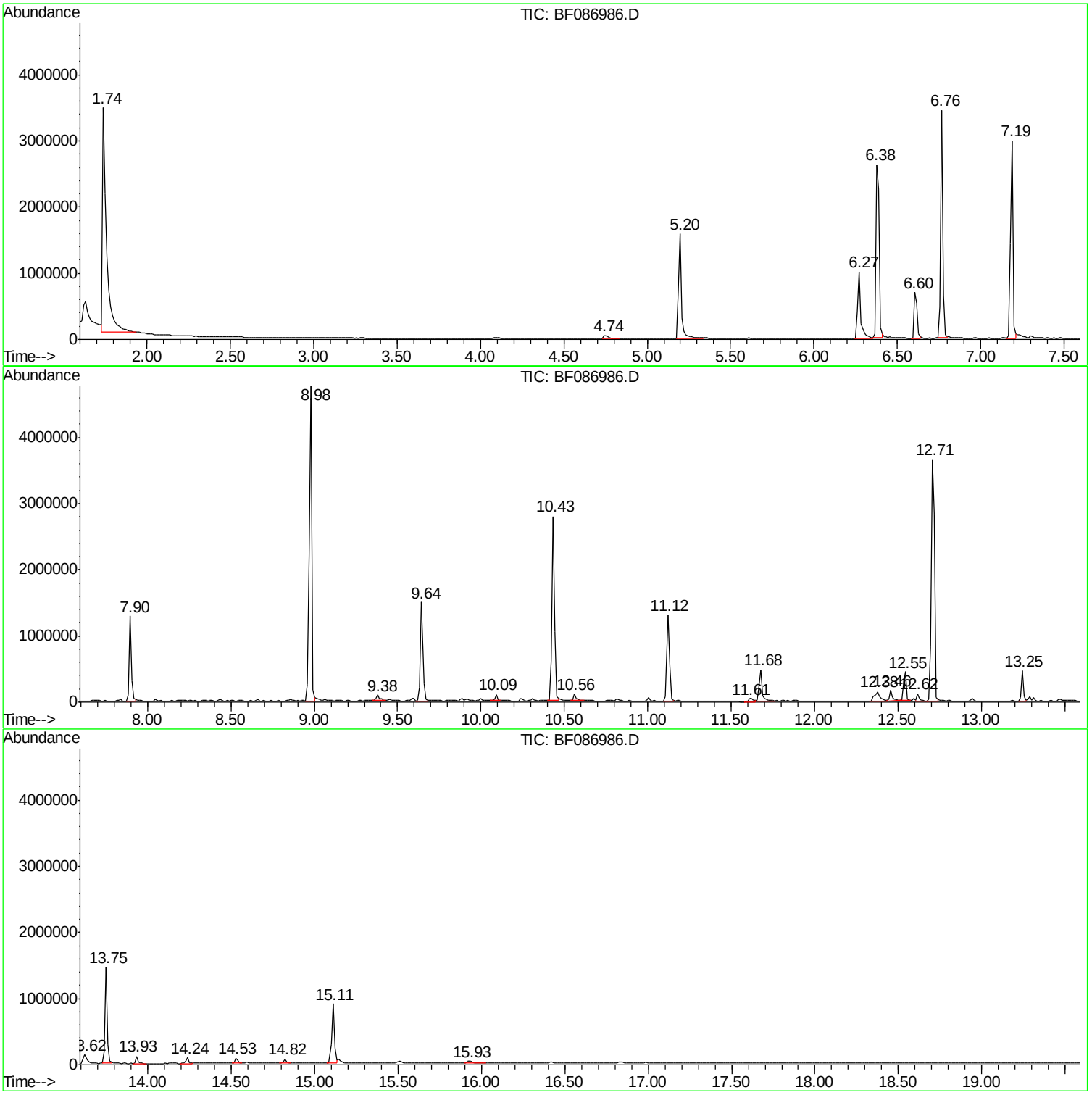
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051316\
Data File : BF086986.D
Acq On : 13 May 2016 22:50
Operator : UM/SJ
Sample : H2877-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051316\
Data File : BF086986.D
Acq On : 13 May 2016 22:50
Operator : UM/SJ
Sample : H2877-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

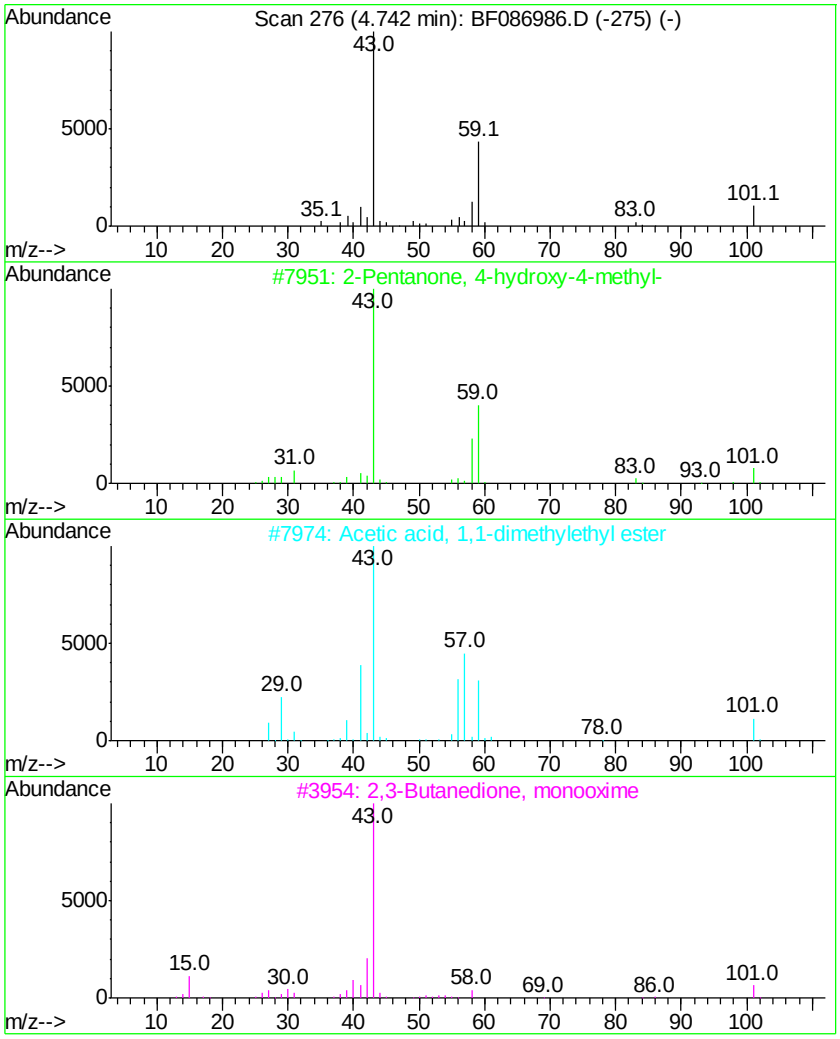
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

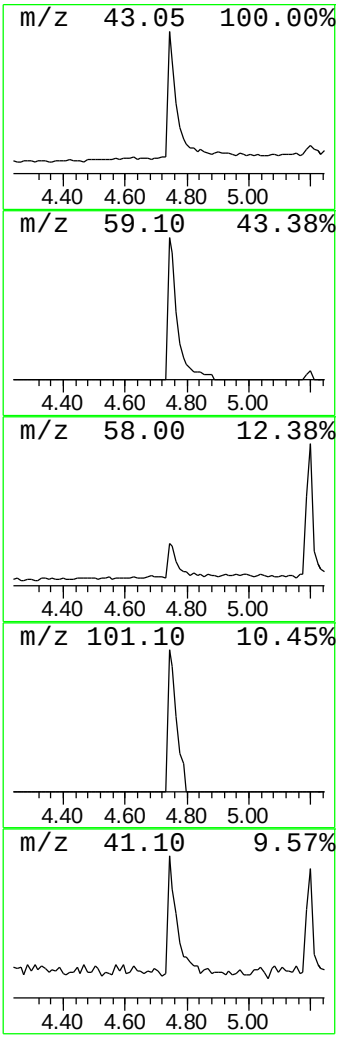
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.74	2.13 ng	96060	1,4-Dichlorobenzene-d4	6.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4	Formamide, N-butyl-	101	C5H11NO	000871-71-6	9
5	Propylamine	59	C3H9N	000107-10-8	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF051316\
Data File : BF086986.D
Acq On : 13 May 2016 22:50
Operator : UM/SJ
Sample : H2877-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

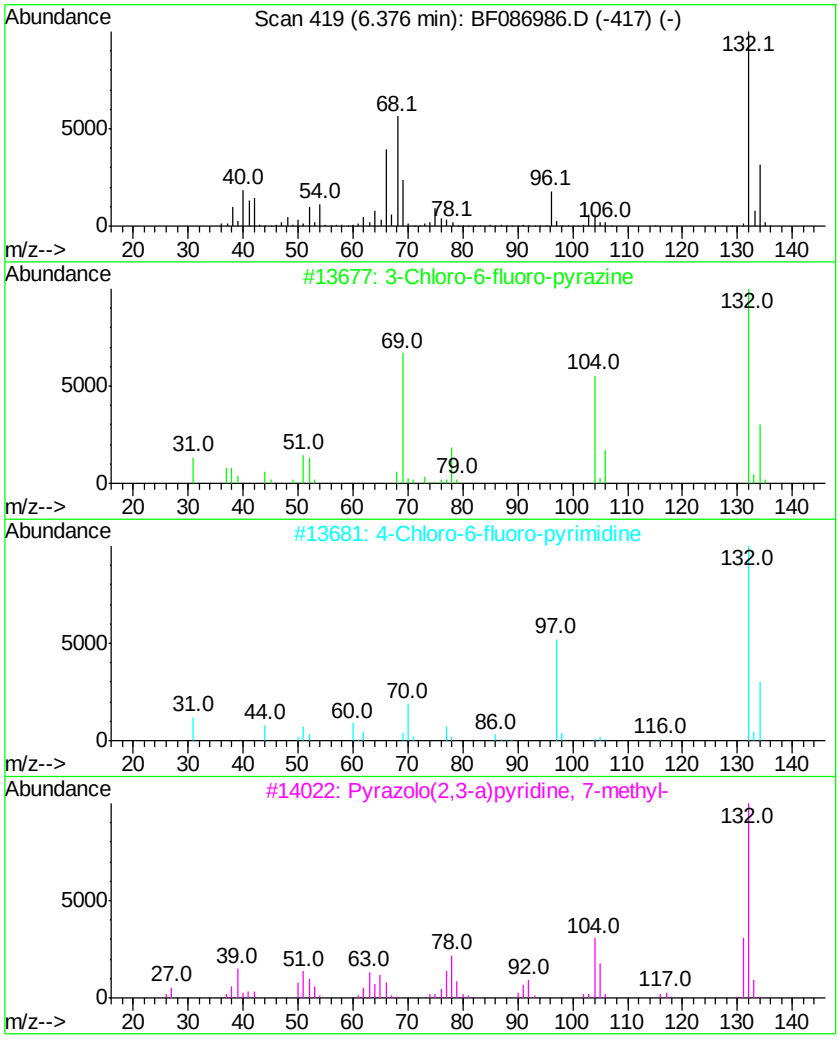
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

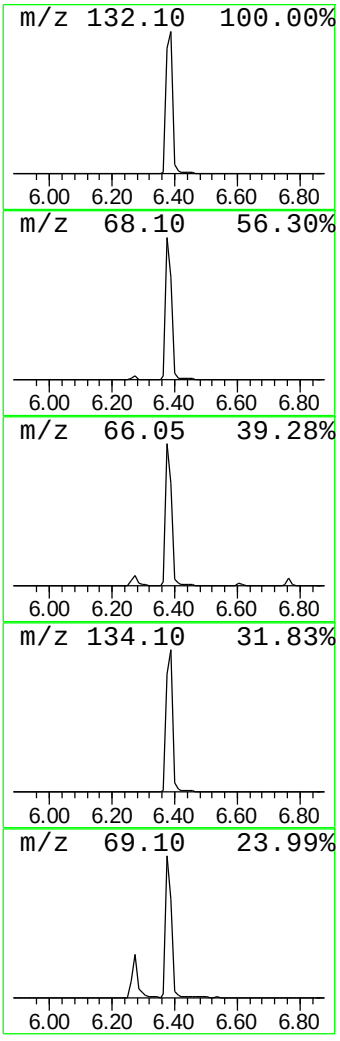
****

Peak Number 3 unknown6.38 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.38	77.66 ng	3502160	1,4-Dichlorobenzene-d4	6.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	14
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF051316\
Data File : BF086986.D
Acq On : 13 May 2016 22:50
Operator : UM/SJ
Sample : H2877-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

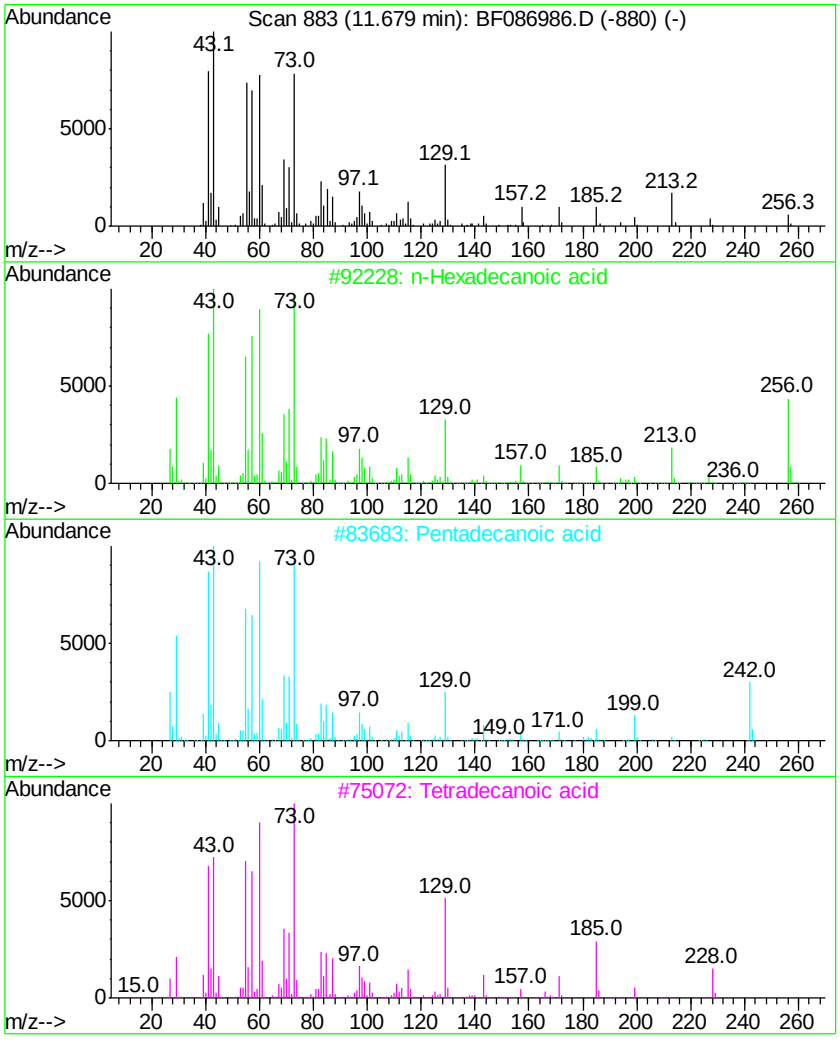
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

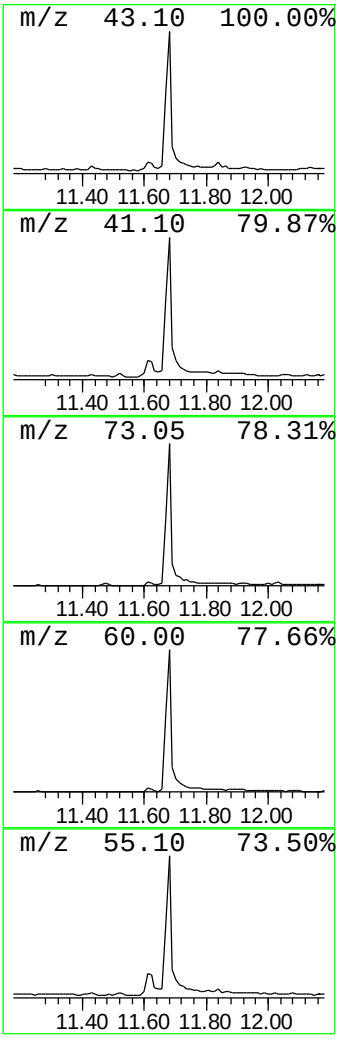
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.68	9.41 ng	617025	Phenanthrene-d10	11.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	49





Data Path : Z:\HPCHEM1\BNA F\DATA\BF051316\
Data File : BF086986.D
Acq On : 13 May 2016 22:50
Operator : UM/SJ
Sample : H2877-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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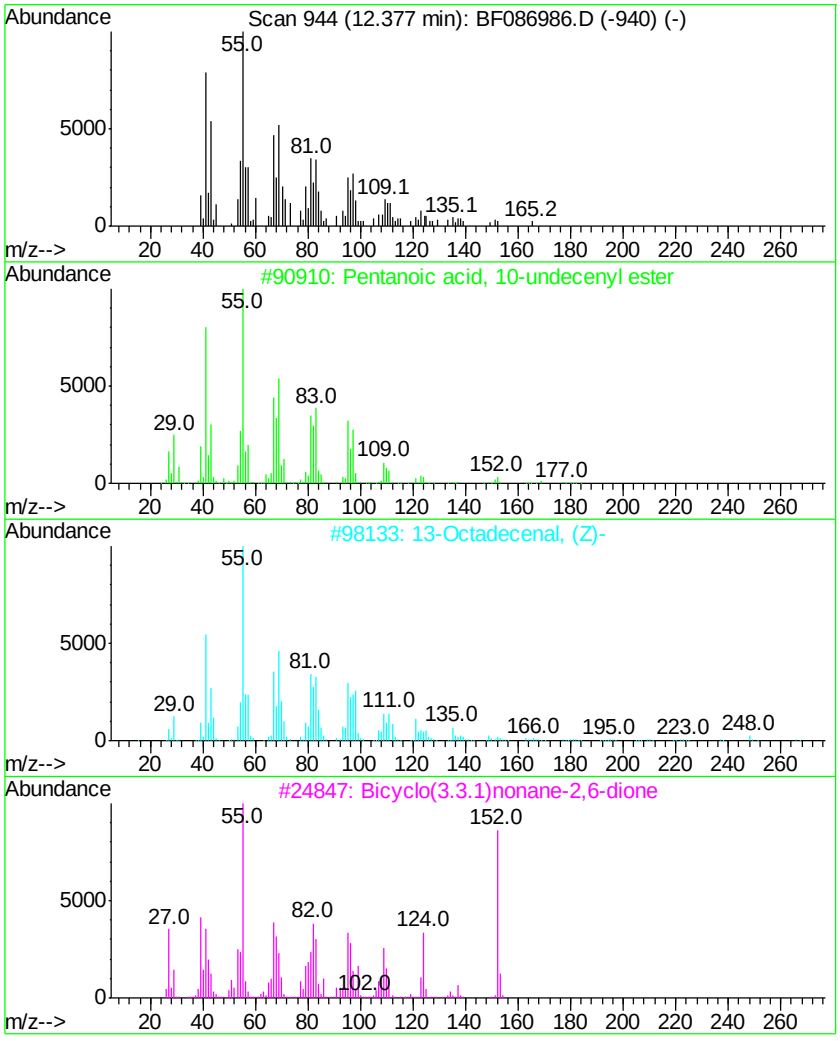
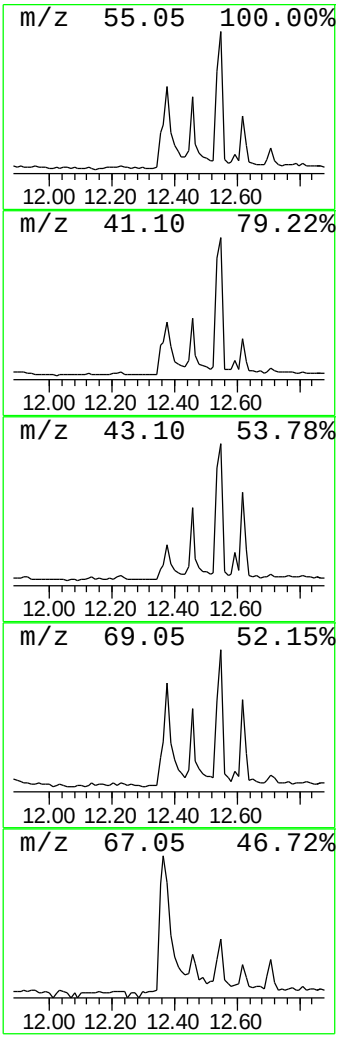
Peak Number 6 Pentanoic acid, 10-undeceny... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.38	5.49 ng	359968	Phenanthrene-d10	11.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid, 10-undecenyl ester	254	C16H30O2	1000159-93-4	86
2	13-Octadecenal, (Z)-	266	C18H34O	058594-45-9	52
3	Bicyclo(3.3.1)nonane-2,6-dione	152	C9H12O2	016473-11-3	52
4	E-1,6-Undecadiene	152	C11H20	1000245-71-2	49
5	cis-7-Dodecen-1-ol	184	C12H24O	020056-92-2	49





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Data File : BF086986.D
Acq On : 13 May 2016 22:50
Operator : UM/SJ
Sample : H2877-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

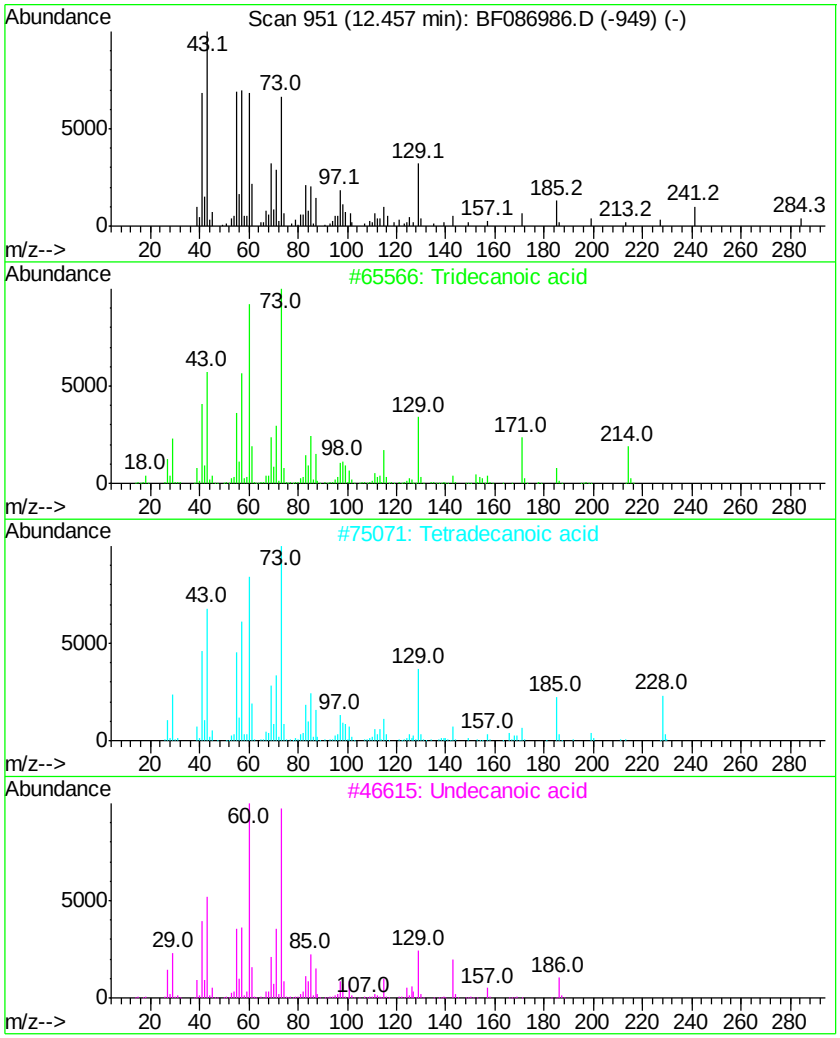
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

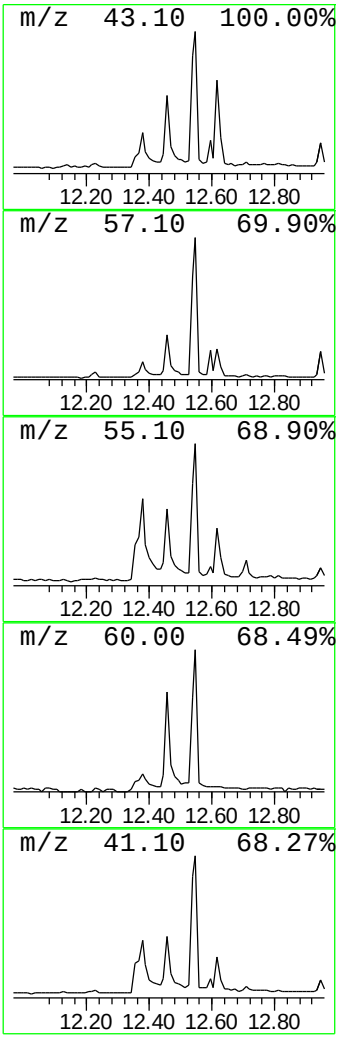
****

Peak Number 7 Tridecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.46	3.08 ng	207508	Chrysene-d12	13.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	64
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3	Undecanoic acid	186	C11H22O2	000112-37-8	53
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	50
5	n-Decanoic acid	172	C10H20O2	000334-48-5	38





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Data File : BF086986.D
Acq On : 13 May 2016 22:50
Operator : UM/SJ
Sample : H2877-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

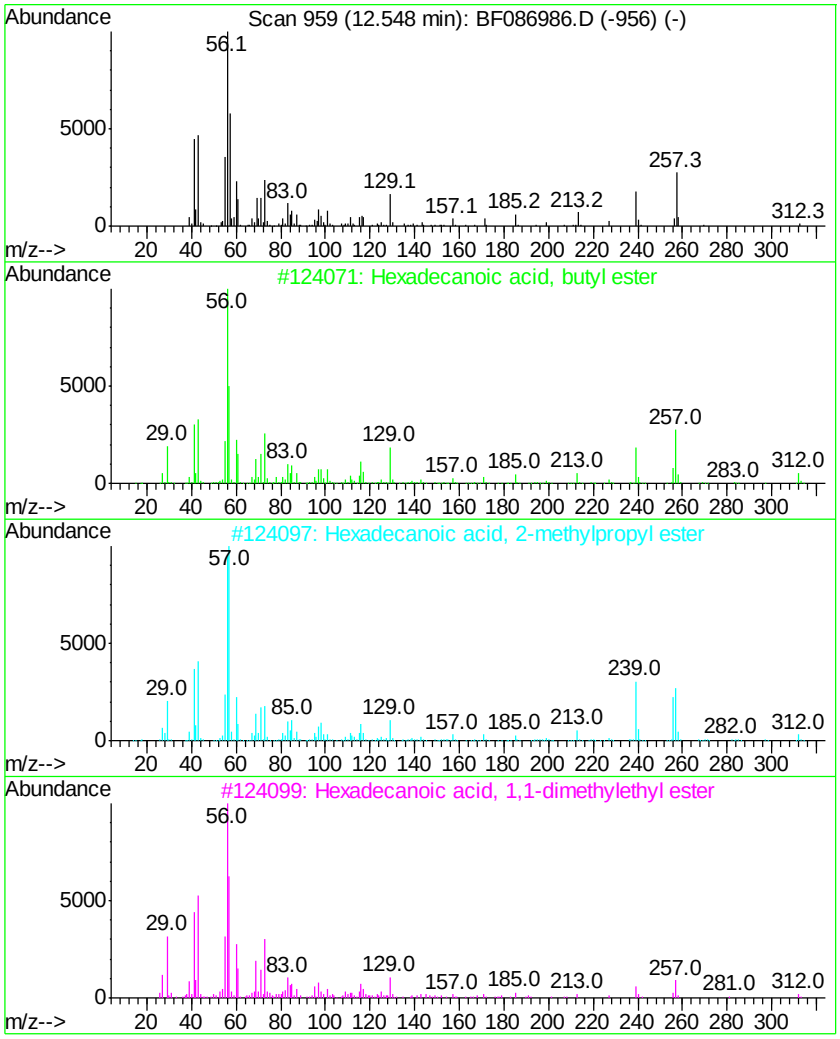
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

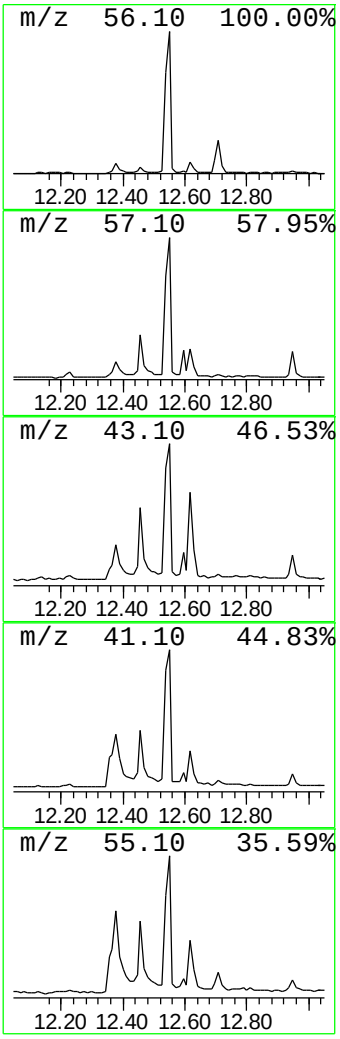
****

Peak Number 8 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.55	7.34 ng	494438	Chrysene-d12	13.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	50
3	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	38
4	2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	37
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051316\
Data File : BF086986.D
Acq On : 13 May 2016 22:50
Operator : UM/SJ
Sample : H2877-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

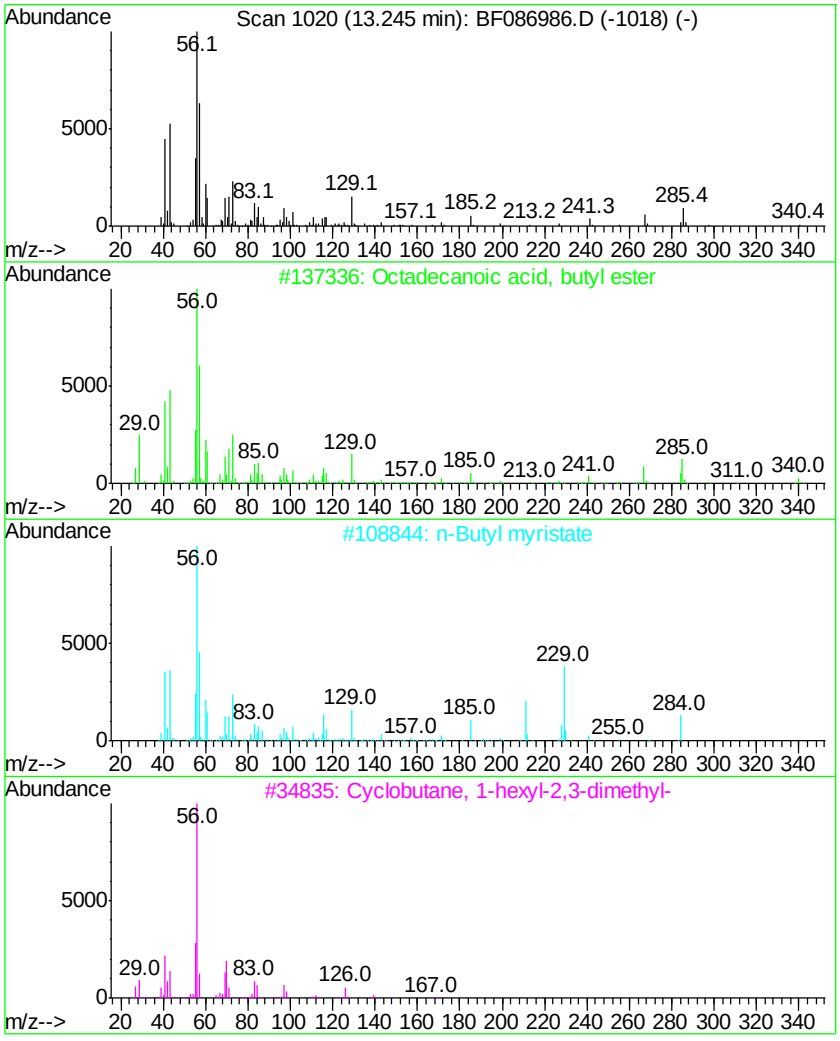
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

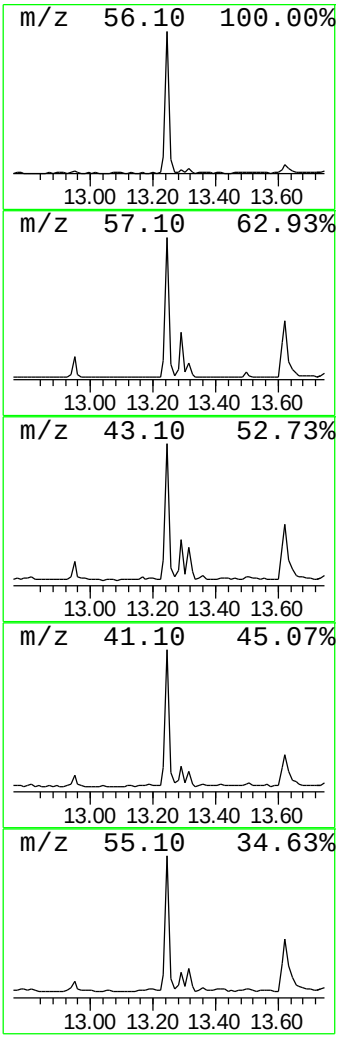
****

Peak Number 9 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.25	5.87 ng	395838	Chrysene-d12	13.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2	n-Butyl myristate	284	C18H36O2	000110-36-1	86
3	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	38
4	Octadecanoic acid	284	C18H36O2	000057-11-4	38
5	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38





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Operator : UM/SJ
Sample : H2877-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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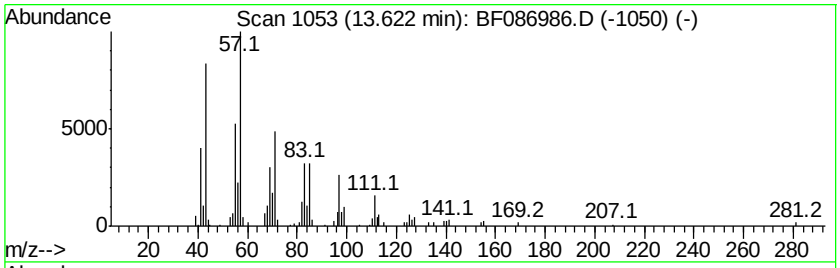
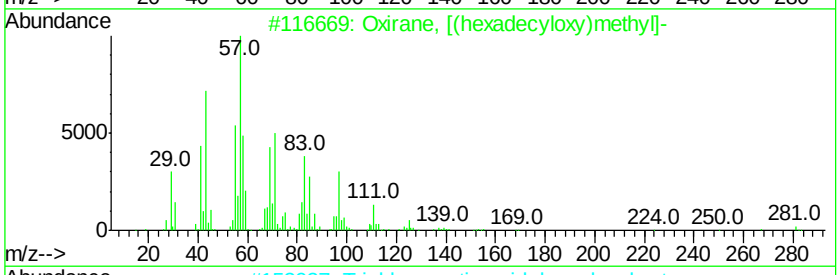
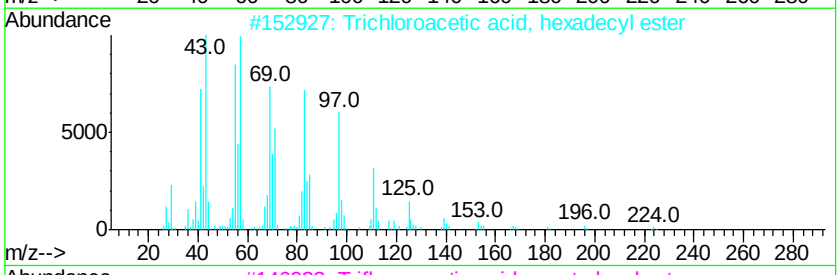
Peak Number 10 Oxirane, [(hexadecyloxy)met... Concentration Rank 8

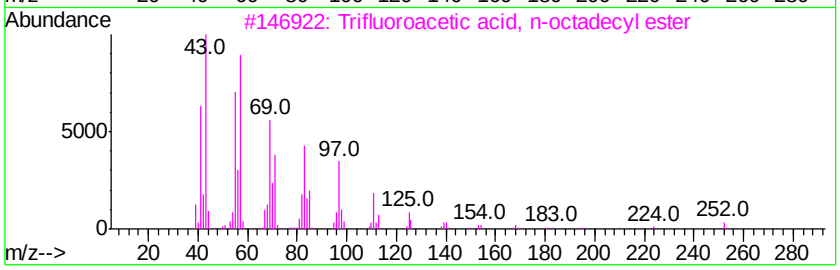
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.62	3.16 ng	213322	Chrysene-d12	13.75

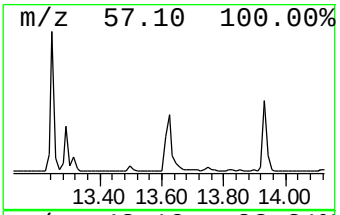
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(hexadecyloxy)methyl]-	298	C19H38O2	015965-99-8	83
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	62
3	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	62
4	17-Pentatriacontene	491	C35H70	006971-40-0	62
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	58

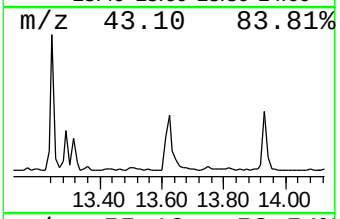


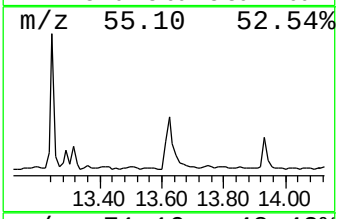


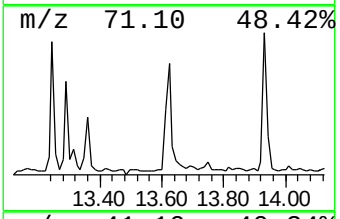


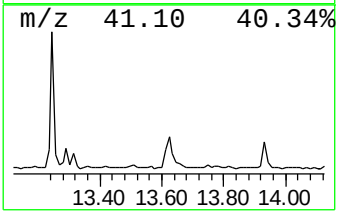












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051316\
Data File : BF086986.D
Acq On : 13 May 2016 22:50
Operator : UM/SJ
Sample : H2877-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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
2-Pentanone, 4-hy...	4.74	2.1	ng	96060	1	6.62	901864	20.0
unknown6.38	6.38	77.7	ng	3502160	1	6.62	901864	20.0
n-Hexadecanoic acid	11.68	9.4	ng	617025	4	11.12	1311420	20.0
Pentanoic acid, 1...	12.38	5.5	ng	359968	4	11.12	1311420	20.0
Tridecanoic acid	12.46	3.1	ng	207508	5	13.75	1348060	20.0
Hexadecanoic acid...	12.55	7.3	ng	494438	5	13.75	1348060	20.0
Octadecanoic acid...	13.25	5.9	ng	395838	5	13.75	1348060	20.0
Oxirane, [(hexade...	13.62	3.2	ng	213322	5	13.75	1348060	20.0