LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111116\
Data File : BF091151.D
Acq On : 11 Nov 2016 20:19
Operator : UM/SJ
Sample : H5609-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-15R

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-BF110316.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	1.744	3	5	62	rVB	3754493	10830278	100.00%	23.658%
2	4.773	268	270	280	rBV	217856	340196	3.14%	0.743%
3	5.242	309	311	329	rBV	1182880	1879534	17.35%	4.106%
4	6.304	402	404	412	rBV	871227	1238937	11.44%	2.706%
5	6.419	412	414	427	rVB	3241036	3880433	35.83%	8.476%
6	6.636	432	433	436	rBV	586282	891075	8.23%	1.946%
7	6.796	445	447	450	rBV	3437177	3159396	29.17%	6.901%
8	7.219	481	484	486	rBV	2446235	2918594	26.95%	6.375%
9	7.928	544	546	553	rBV	1396389	1329465	12.28%	2.904%
10	9.013	638	641	643	rBV	4813668	5327082	49.19%	11.636%
11	9.139	650	652	654	rVB	121197	112886	1.04%	0.247%
12	9.631	692	695	697	rVV3	82891	150695	1.39%	0.329%
13	9.676	697	699	701	rVV	1763855	1484839	13.71%	3.243%
14	10.065	729	733	736	rBV3	55380	131624	1.22%	0.288%
15	10.122	736	738	740	rVB	120946	118533	1.09%	0.259%
16	10.465	766	768	771	rBV	2771390	3012681	27.82%	6.581%
17	10.591	777	779	783	rVB2	129754	182024	1.68%	0.398%
18	11.151	826	828	831	rBV	1087629	1218669	11.25%	2.662%
19	11.711	874	877	884	rBV	520205	777894	7.18%	1.699%
20	11.825	884	887	893	rVB	69382	130608	1.21%	0.285%
21	12.488	942	945	951	rBV	548057	629281	5.81%	1.375%
22	12.739	964	967	970	rBV	4202259	3950593	36.48%	8.630%
23	13.642	1043	1046	1049	rBV	132069	154045	1.42%	0.336%
24	13.711	1049	1052	1056	rVV	144450	320792	2.96%	0.701%
25	13.780	1056	1058	1063	rVB	801902	834820	7.71%	1.824%
26	15.151	1175	1178	1188	rVB	649349	774484	7.15%	1.692%

Sum of corrected areas: 45779458

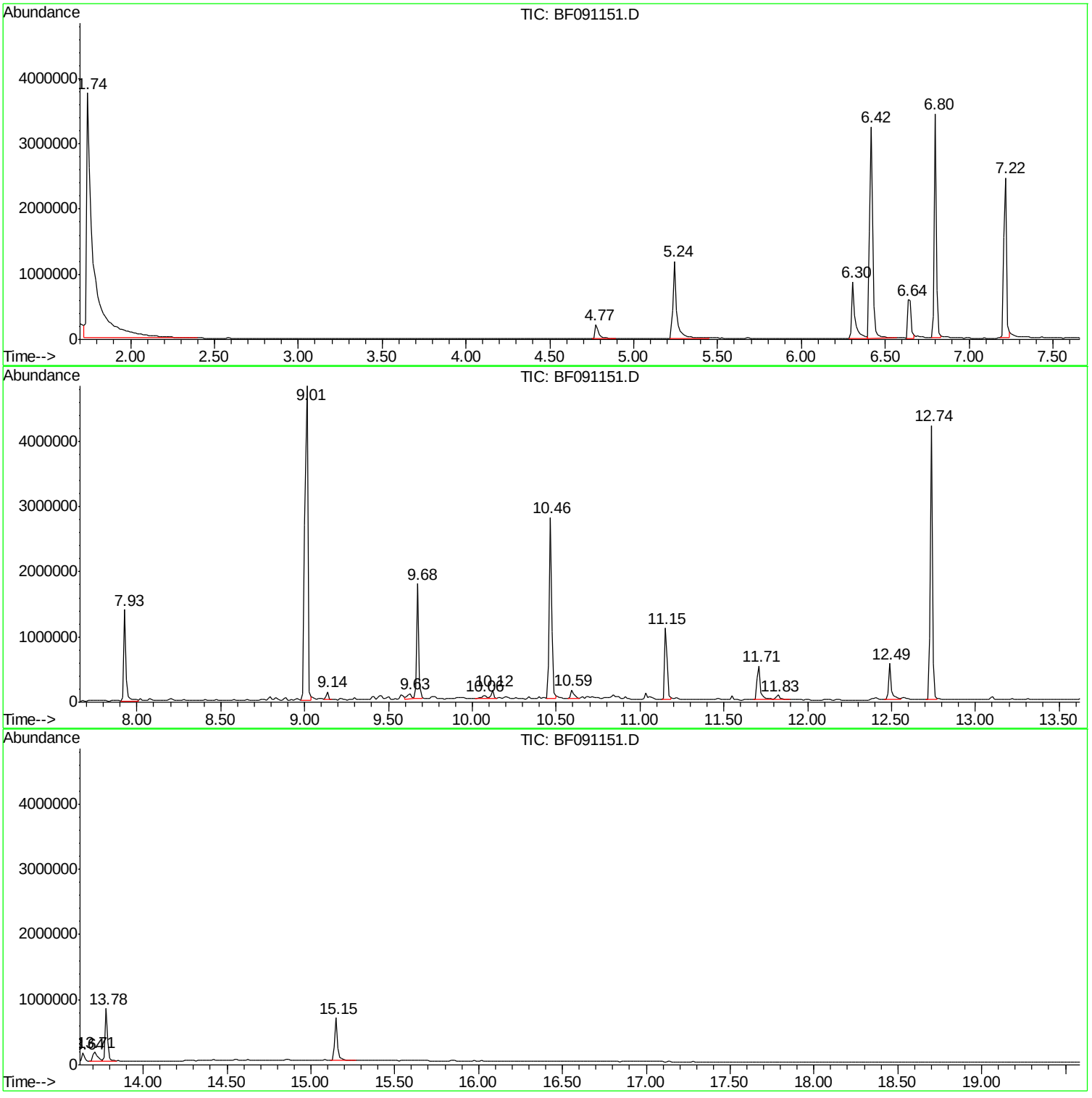
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111116\
Data File : BF091151.D
Acq On : 11 Nov 2016 20:19
Operator : UM/SJ
Sample : H5609-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-15R

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.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\BF111116\
Data File : BF091151.D
Acq On : 11 Nov 2016 20:19
Operator : UM/SJ
Sample : H5609-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-15R

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

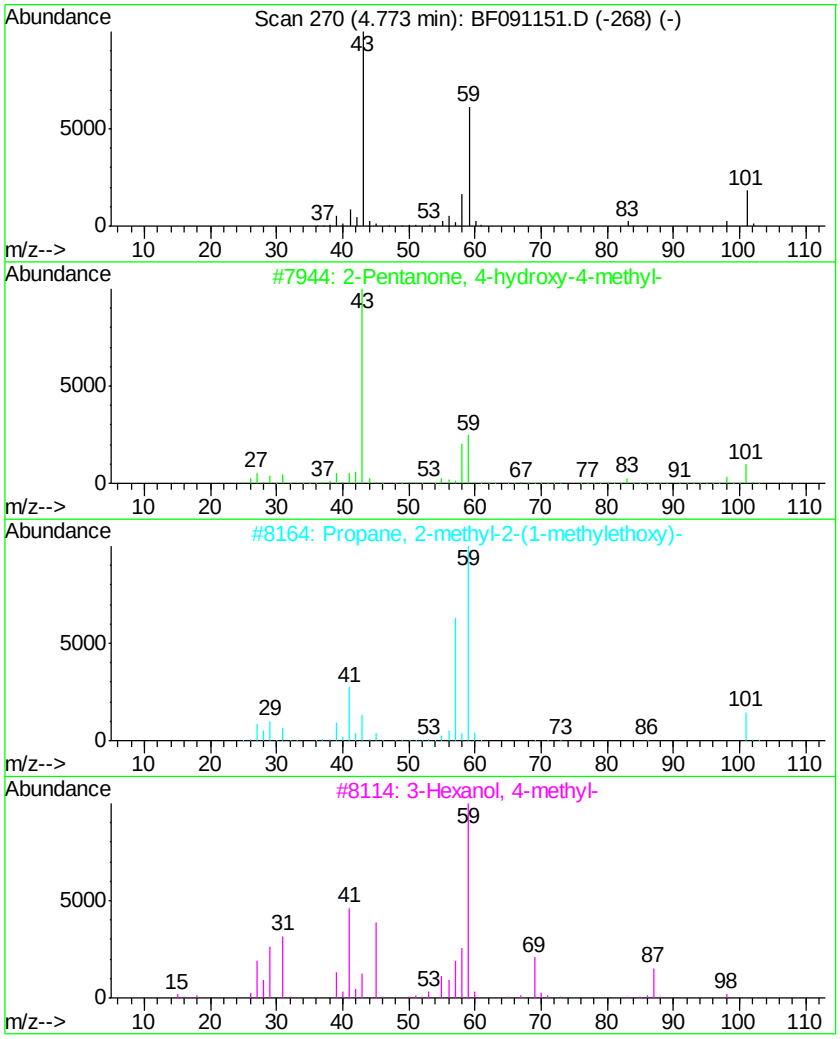
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

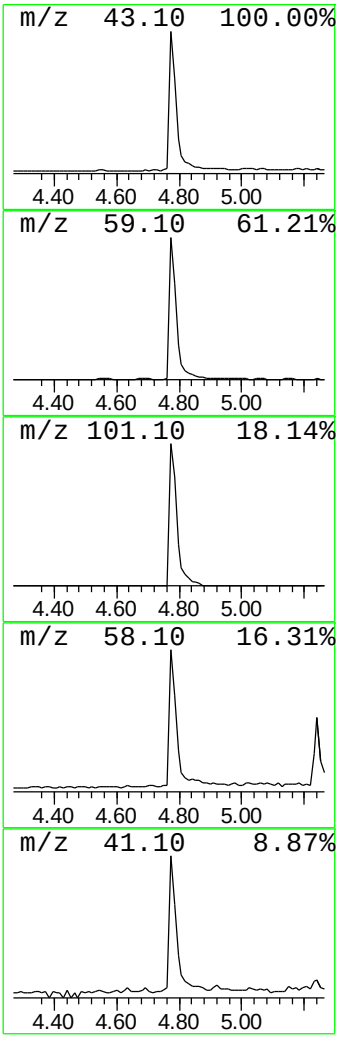
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.77	7.64 ng	340196	1,4-Dichlorobenzene-d4	6.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Library Search Compound Report

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Data File : BF091151.D
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Operator : UM/SJ
Sample : H5609-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-15R

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.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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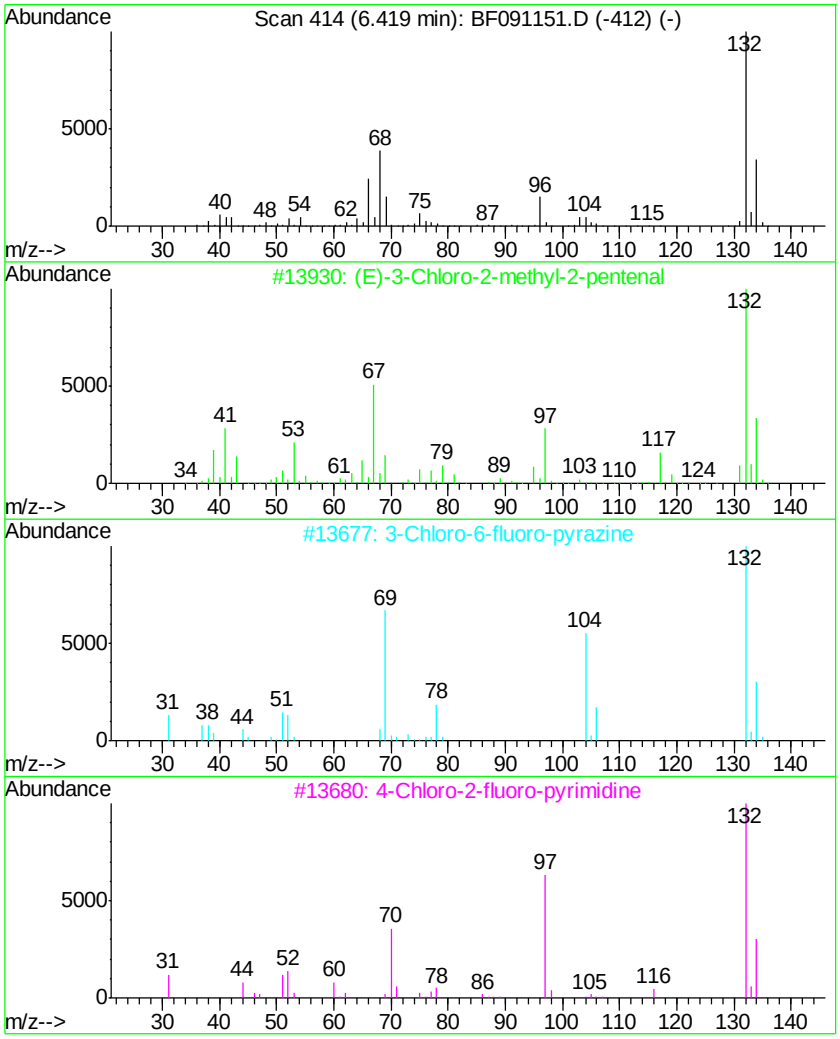
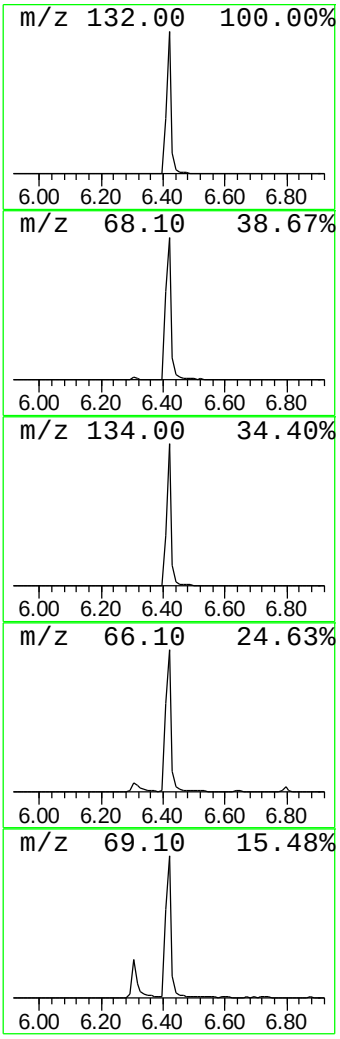
Peak Number 3 unknown6.42 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	87.10 ng	3880430	1,4-Dichlorobenzene-d4	6.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Library Search Compound Report

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Sample : H5609-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-15R

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
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TIC Library : C:\DATABASE\NIST02.L
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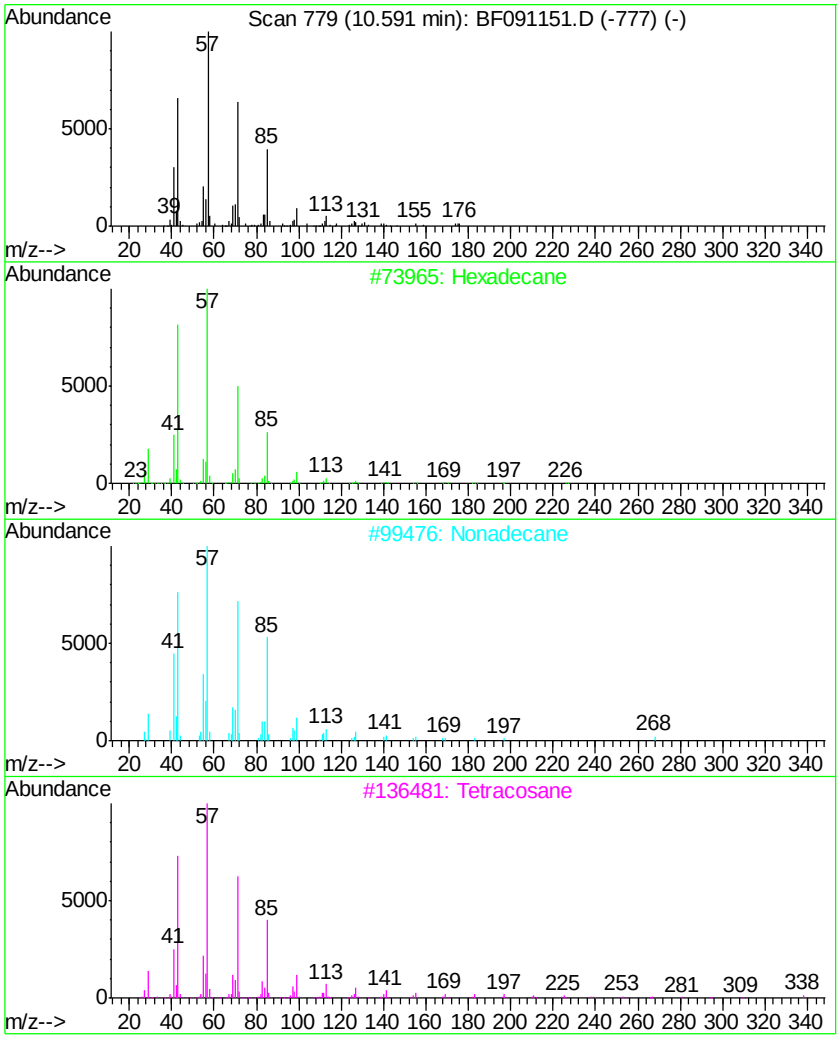
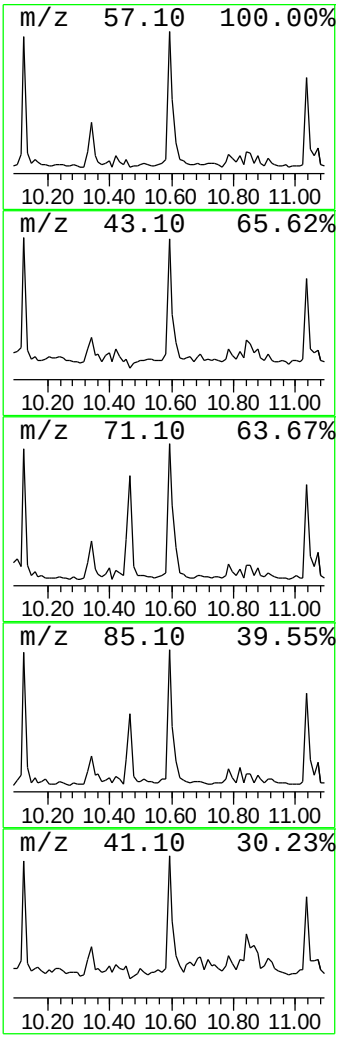
Peak Number 5 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.59	2.99 ng	182024	Phenanthrene-d10	11.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Nonadecane	268	C19H40	000629-92-5	86
3	Tetracosane	338	C24H50	000646-31-1	83
4	Heptacosane	380	C27H56	000593-49-7	78
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	78





Library Search Compound Report

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Sample : H5609-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-15R

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

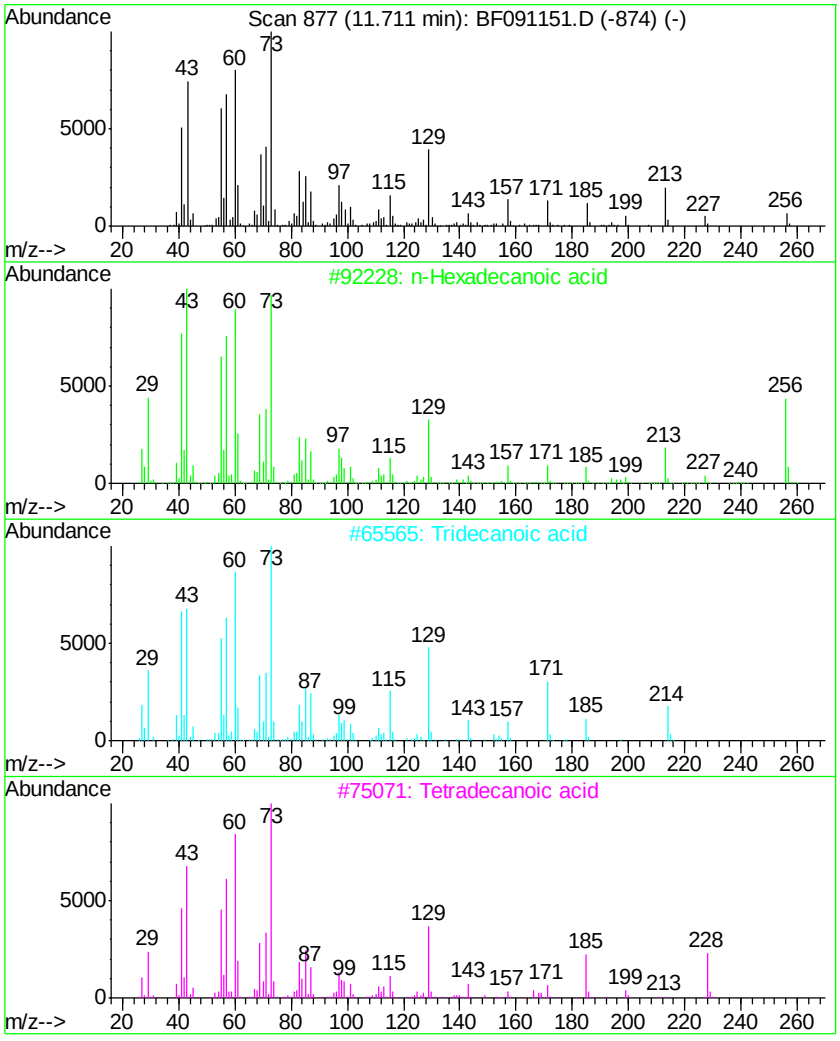
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

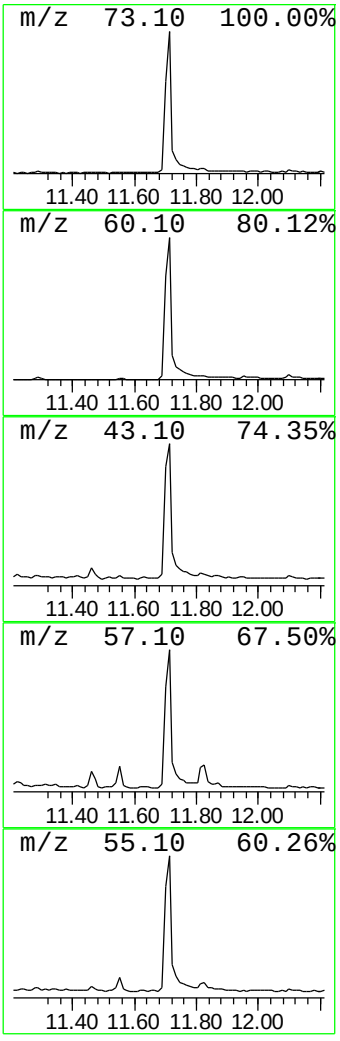
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.71	12.77 ng	777894	Phenanthrene-d10	11.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	30





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111116\
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Operator : UM/SJ
Sample : H5609-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-15R

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

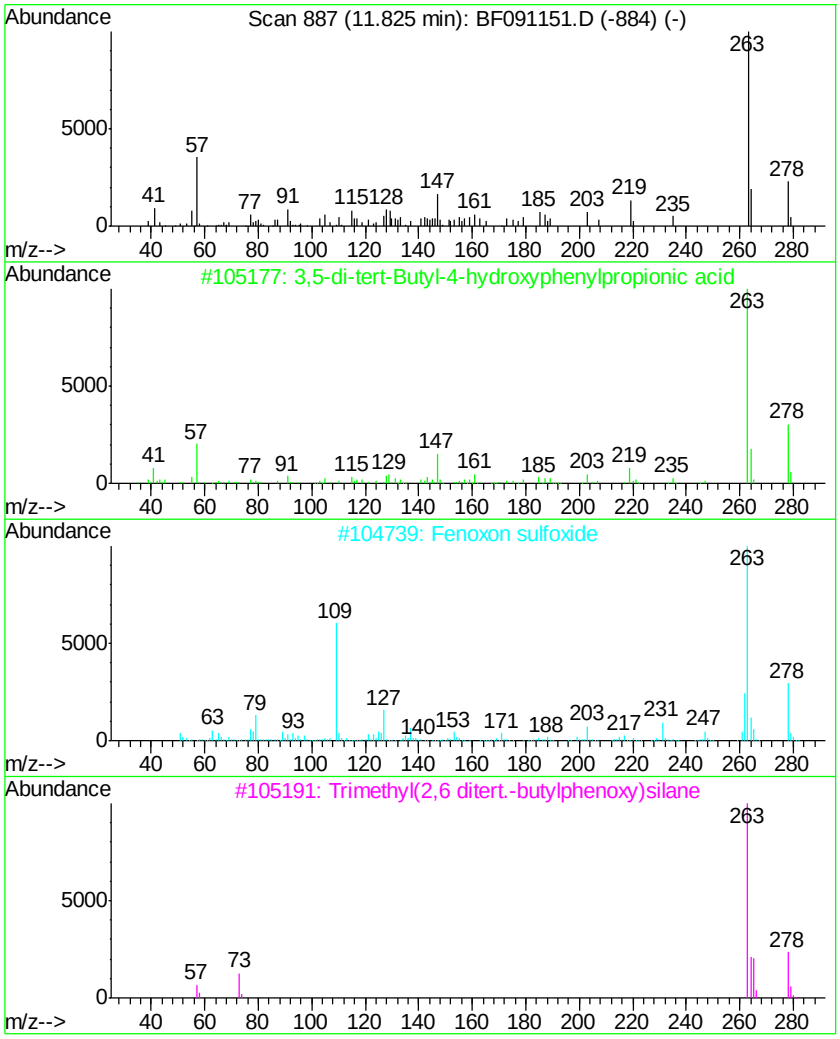
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

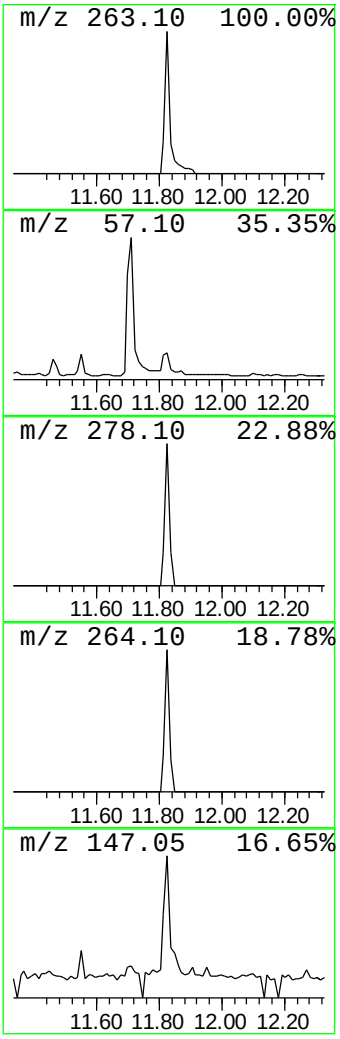
****

Peak Number 7 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.83	2.14 ng	130608	Phenanthrene-d10	11.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-di-tert-Butyl-4-hydroxyphenyl...	278	C17H26O3	020170-32-5	97
2	Fenoxon sulfoxide	278	C10H15O5PS	006552-13-2	59
3	Trimethyl(2,6 ditert.-butylpheno...	278	C17H30OSi	010416-73-6	59
4	Ethanone, [1-(2,5-diphenyl-2H-1,...	263	C16H13N3O	322647-34-7	47
5	Benzoic acid, 3,5-bis(1,1-dimeth...	278	C17H26O3	001620-64-0	45





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111116\
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Sample : H5609-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-15R

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

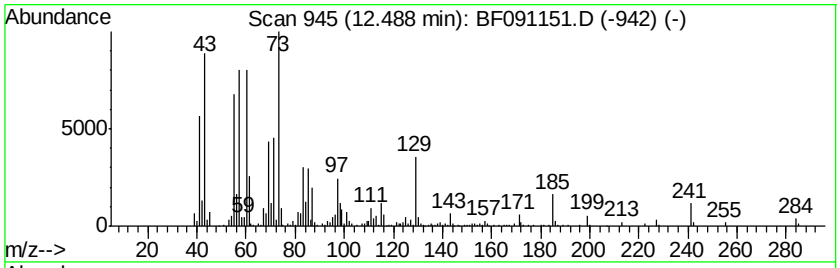
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

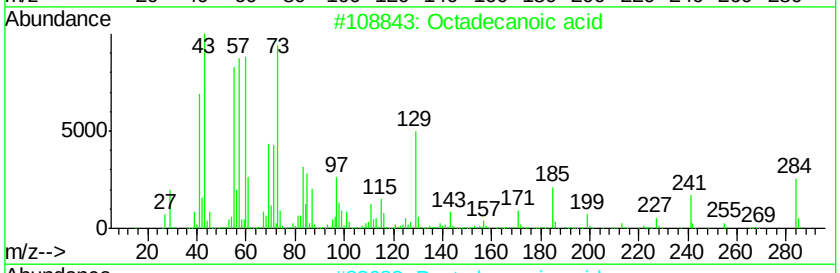
****

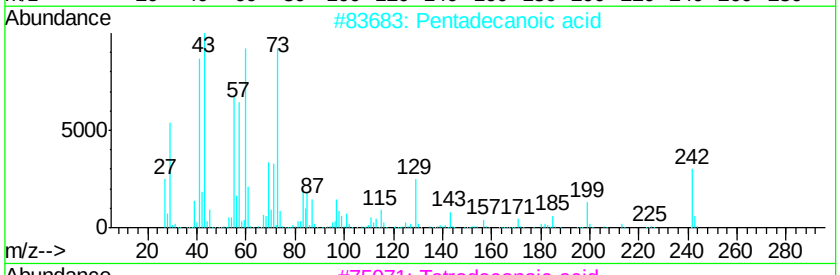
Peak Number 8 Octadecanoic acid Concentration Rank 4

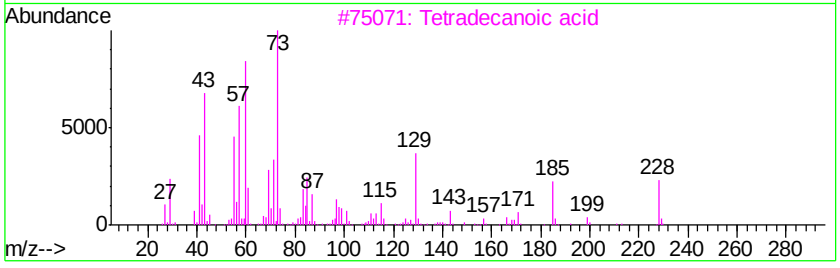
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	15.08 ng	629281	Chrysene-d12	13.78

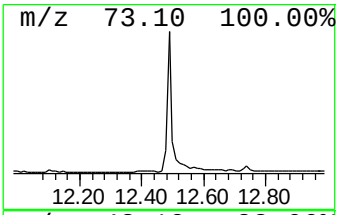
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4	N-Cyclooct-4-enylacetamide	167	C10H17NO	170952-69-9	30
5	Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	20

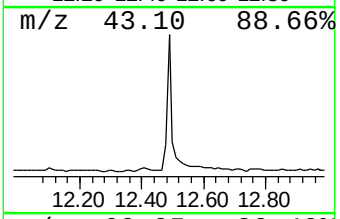


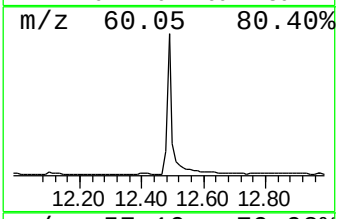


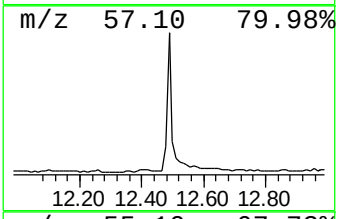


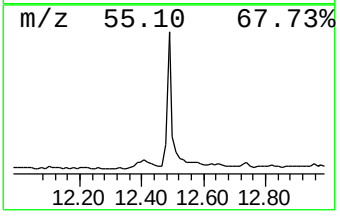












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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

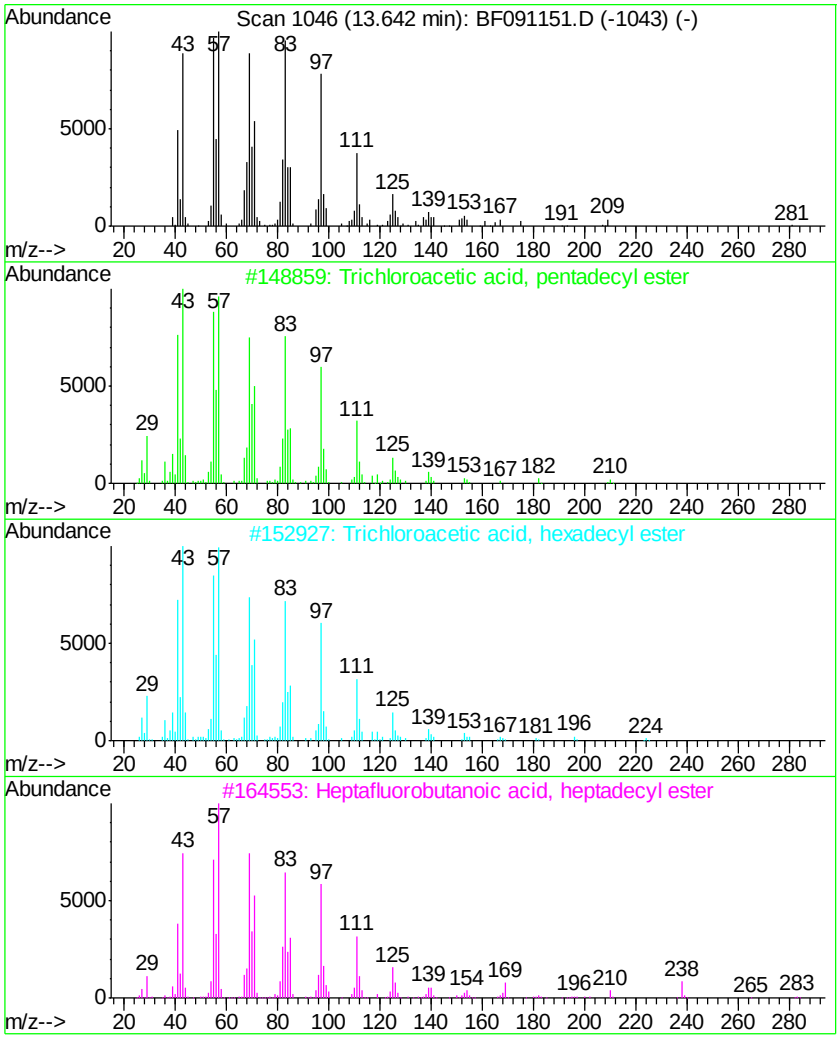
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

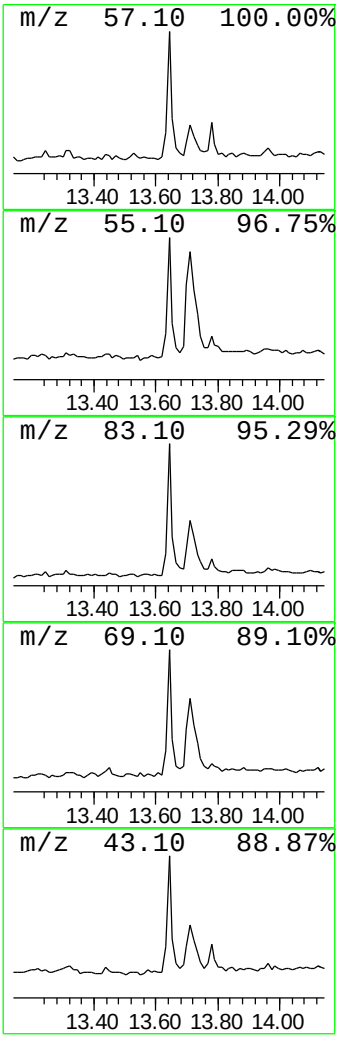
****

Peak Number 9 Trichloroacetic acid, penta... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.64	3.69 ng	154045	Chrysene-d12	13.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	93
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91





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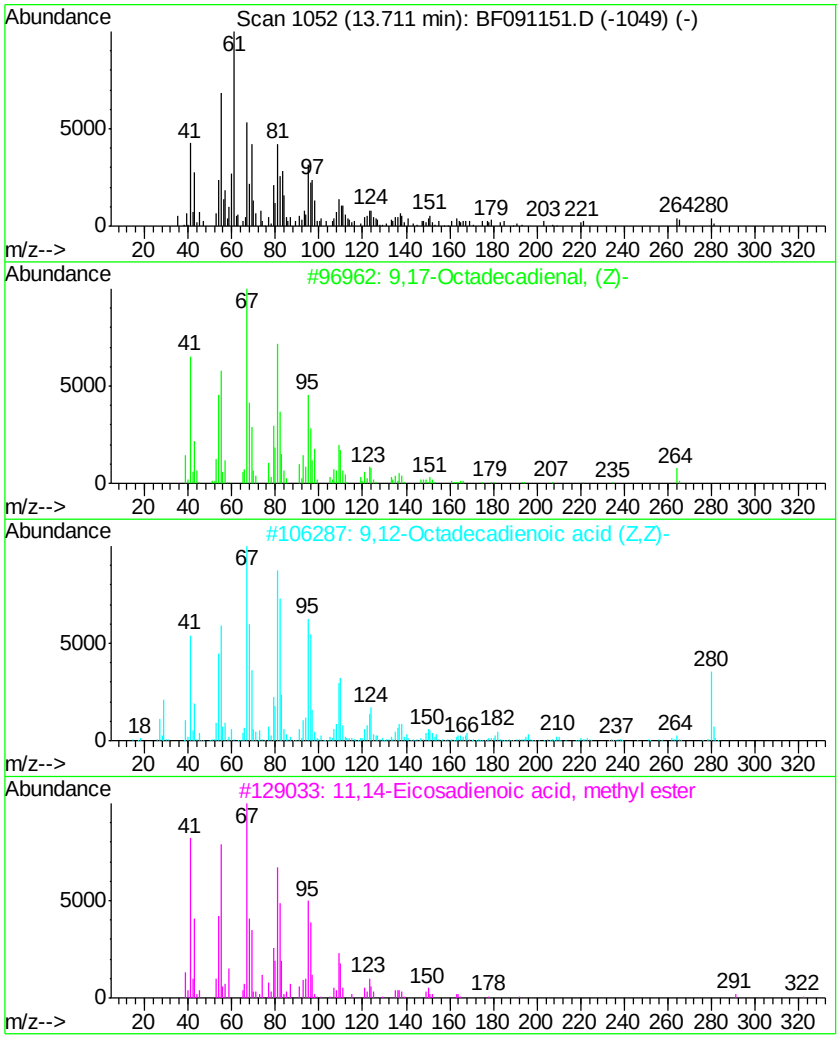
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

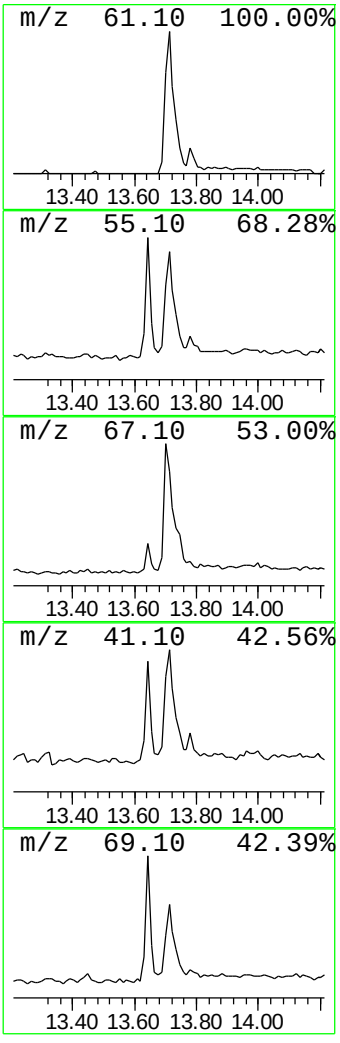
****

Peak Number 10 9,17-Octadecadienal, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	7.69 ng	320792	Chrysene-d12	13.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,17-Octadecadienal, (Z)-	264	C18H32O	056554-35-9	93
2	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	93
3	11,14-Eicosadienoic acid, methyl...	322	C21H38O2	002463-02-7	38
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	38
5	7,11-Hexadecadienal	236	C16H28O	1000130-85-7	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111116\
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Operator : UM/SJ
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Instrument : BNA_F
ClientSampleId : MW-15R

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.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...	4.77	7.6	ng	340196	1	6.65	891075	20.0
unknown6.42	6.42	87.1	ng	3880430	1	6.65	891075	20.0
Hexadecane	10.59	3.0	ng	182024	4	11.15	1218670	20.0
n-Hexadecanoic acid	11.71	12.8	ng	777894	4	11.15	1218670	20.0
3,5-di-tert-Butyl...	11.83	2.1	ng	130608	4	11.15	1218670	20.0
Octadecanoic acid	12.49	15.1	ng	629281	5	13.78	834820	20.0
Trichloroacetic a...	13.64	3.7	ng	154045	5	13.78	834820	20.0
9,17-Octadecadien...	13.71	7.7	ng	320792	5	13.78	834820	20.0