LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112515\
Data File : BF083270.D
Acq On : 25 Nov 2015 13:29
Operator : UM/IZ
Sample : G4534-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-44

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-BF112115.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	3.976	172	174	180	rBV	65738	135600	2.32%	0.349%
2	4.707	235	238	247	rBV	676563	1048358	17.90%	2.700%
3	5.176	277	279	292	rBV	1280029	1742379	29.75%	4.487%
4	5.587	313	315	323	rVB	82973	124704	2.13%	0.321%
5	6.250	371	373	380	rBV	1103042	1157543	19.77%	2.981%
6	6.364	380	383	385	rBV	2251795	2958698	50.53%	7.619%
7	6.582	400	402	405	rBV	801735	997076	17.03%	2.567%
8	6.742	414	416	419	rBV	3847763	3898239	66.57%	10.038%
9	7.164	450	453	455	rBV	3037425	3745691	63.97%	9.645%
10	7.873	513	515	518	rBV	1366293	1329037	22.70%	3.422%
11	8.959	607	610	613	rBV	5874619	5855765	100.00%	15.079%
12	9.359	643	645	648	rBV	121637	110387	1.89%	0.284%
13	9.622	666	668	670	rVB	1658997	1546748	26.41%	3.983%
14	10.410	734	737	740	rBV	2669229	2564448	43.79%	6.603%
15	10.548	747	749	752	rVB	62085	75331	1.29%	0.194%
16	10.936	780	783	786	rBV	79217	167307	2.86%	0.431%
17	11.096	795	797	801	rBV	1689541	1620349	27.67%	4.172%
18	11.153	801	802	807	rVB2	45269	71152	1.22%	0.183%
19	11.656	843	846	849	rBV2	546168	568249	9.70%	1.463%
20	11.713	849	851	854	rVB4	34722	69522	1.19%	0.179%
21	12.354	904	907	912	rBV3	35300	82487	1.41%	0.212%
22	12.434	912	914	919	rBV	626341	807699	13.79%	2.080%
23	12.525	920	922	926	rVB	48318	73246	1.25%	0.189%
24	12.685	933	936	939	rBV	4792579	5356329	91.47%	13.792%
25	13.165	973	978	982	rBV6	22264	69405	1.19%	0.179%
26	13.599	1013	1016	1020	rBV2	92926	149919	2.56%	0.386%
27	13.725	1024	1027	1029	rBV	1208482	1456331	24.87%	3.750%
28	14.994	1136	1138	1142	rBV2	38244	64758	1.11%	0.167%
29	15.074	1142	1145	1148	rBV	882710	988357	16.88%	2.545%

Sum of corrected areas: 38835114

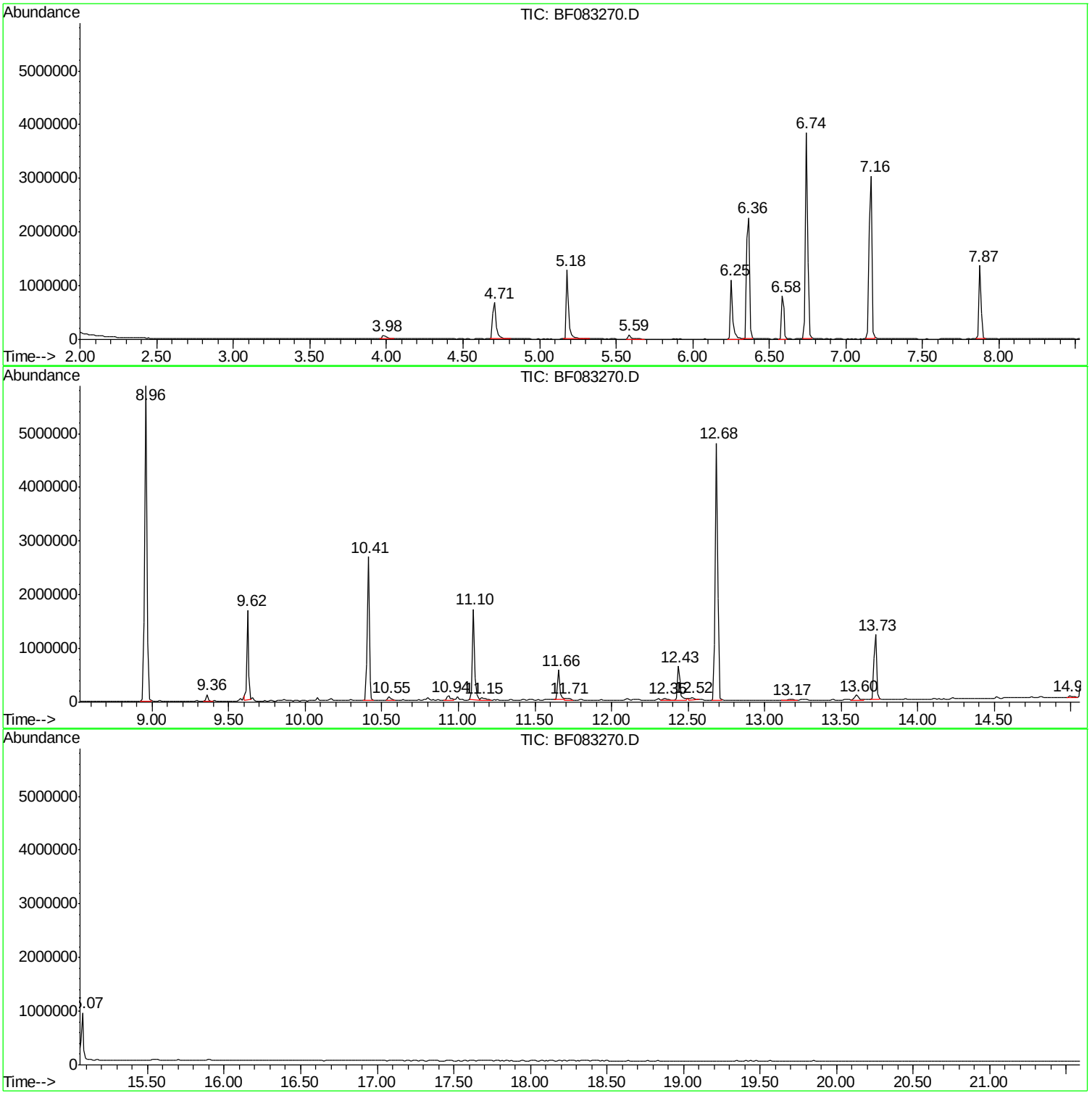
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112515\
Data File : BF083270.D
Acq On : 25 Nov 2015 13:29
Operator : UM/IZ
Sample : G4534-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-44

Quant Method : Z:\HPCHEM1\BNA_F\Methods\8270-BF112115.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\BF112515\
Data File : BF083270.D
Acq On : 25 Nov 2015 13:29
Operator : UM/IZ
Sample : G4534-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-44

Quant Method : Z:\HPCHEM1\BNA_F\Methods\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

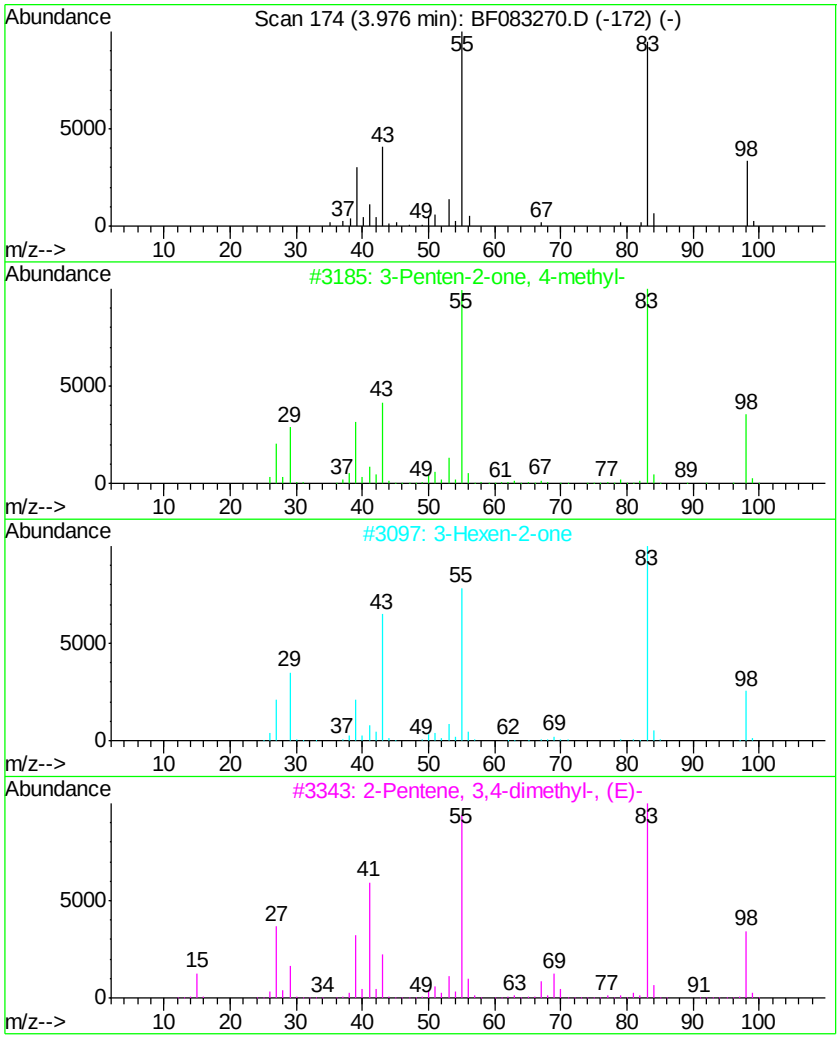
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

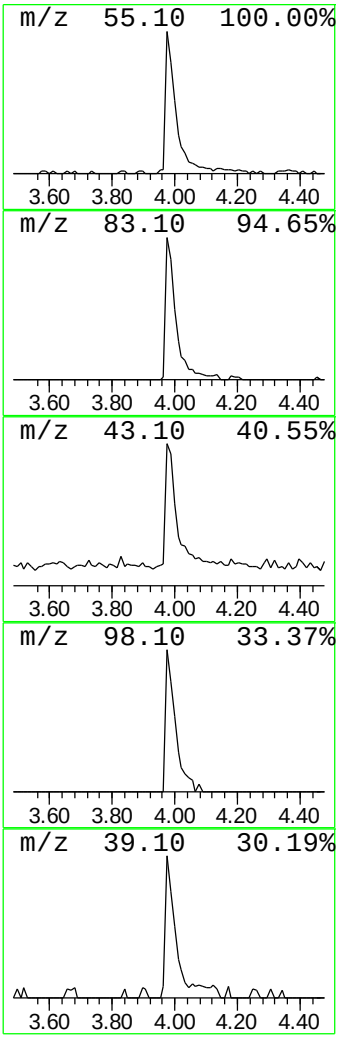
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.98	2.72 ng	135600	1,4-Dichlorobenzene-d4	6.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112515\
Data File : BF083270.D
Acq On : 25 Nov 2015 13:29
Operator : UM/IZ
Sample : G4534-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-44

Quant Method : Z:\HPCHEM1\BNA_F\Methods\8270-BF112115.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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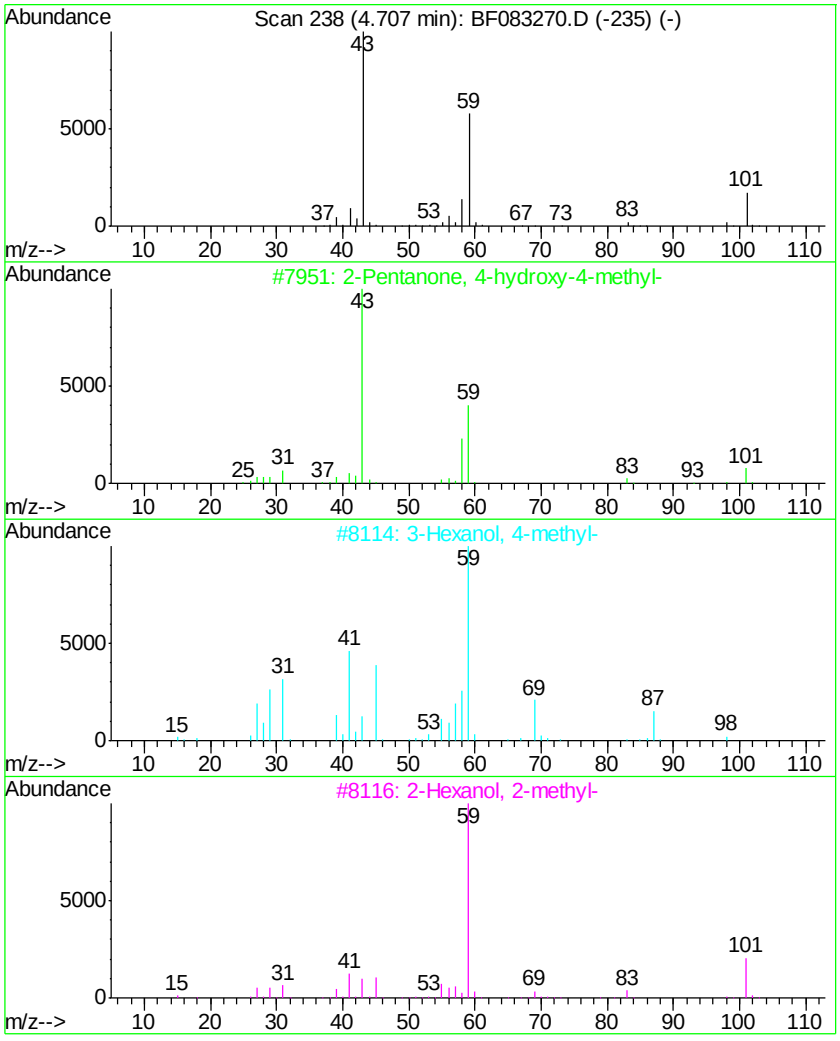
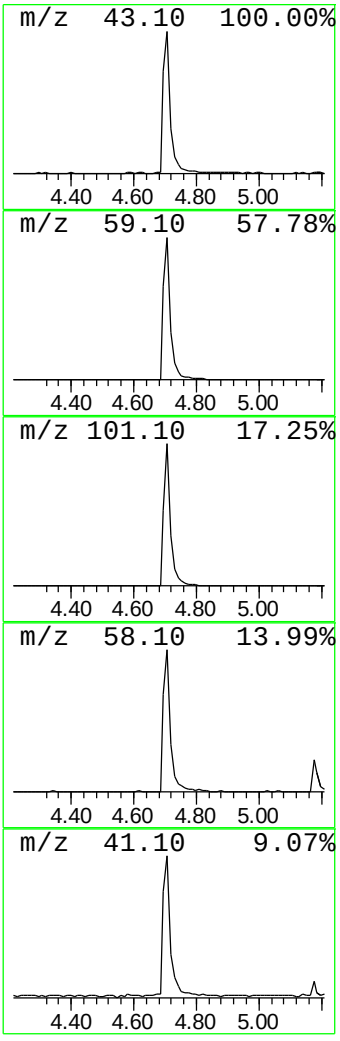
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.71	21.03 ng	1048360	1,4-Dichlorobenzene-d4	6.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112515\
Data File : BF083270.D
Acq On : 25 Nov 2015 13:29
Operator : UM/IZ
Sample : G4534-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-44

Quant Method : Z:\HPCHEM1\BNA_F\Methods\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

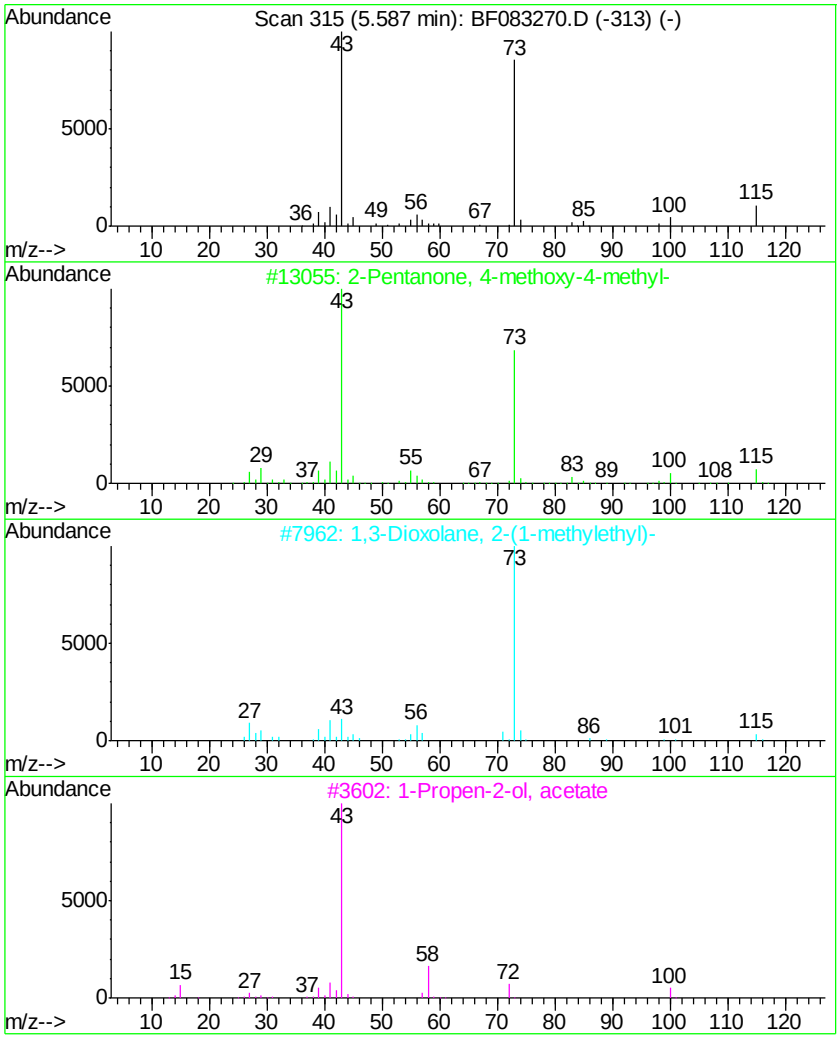
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

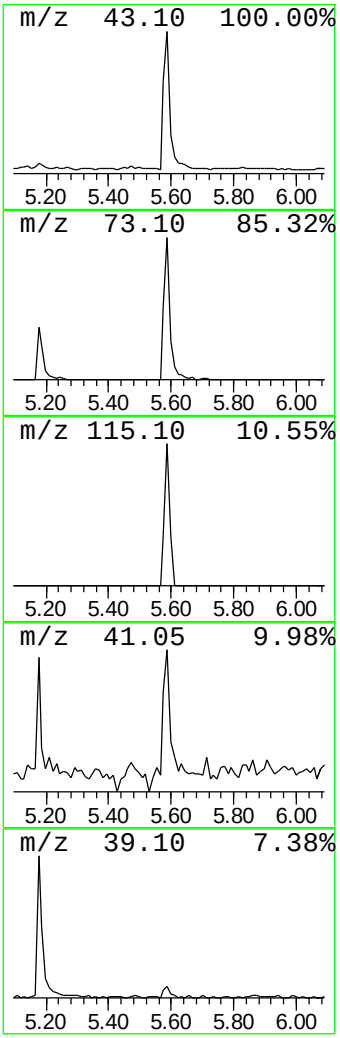
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.59	2.50 ng	124704	1,4-Dichlorobenzene-d4	6.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	64
2	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	17
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	10
5	Hexane, 2-methyl-	100	C7H16	000591-76-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112515\
Data File : BF083270.D
Acq On : 25 Nov 2015 13:29
Operator : UM/IZ
Sample : G4534-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-44

Quant Method : Z:\HPCHEM1\BNA_F\Methods\8270-BF112115.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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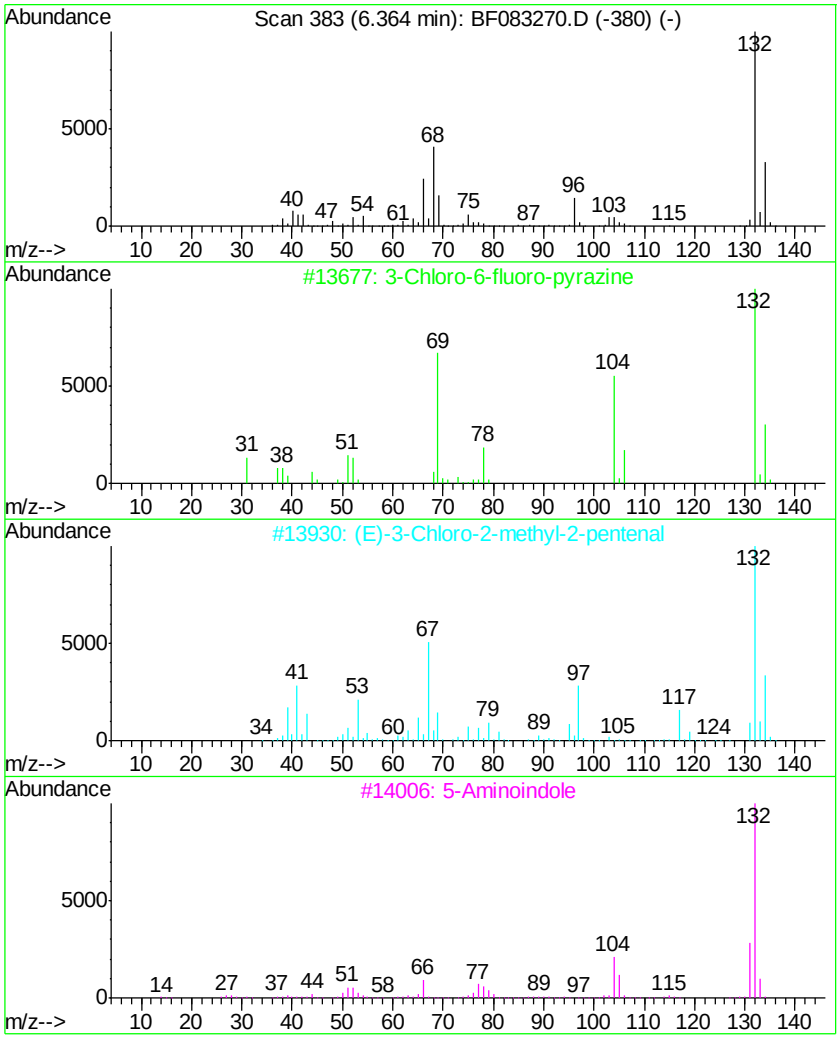
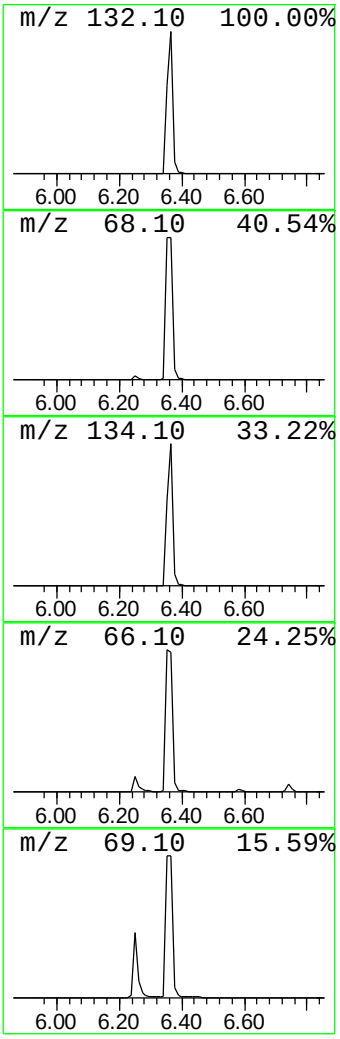
Peak Number 4 unknown6.36 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	59.35 ng	2958700	1,4-Dichlorobenzene-d4	6.58

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	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	10
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112515\
Data File : BF083270.D
Acq On : 25 Nov 2015 13:29
Operator : UM/IZ
Sample : G4534-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-44

Quant Method : Z:\HPCHEM1\BNA_F\Methods\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

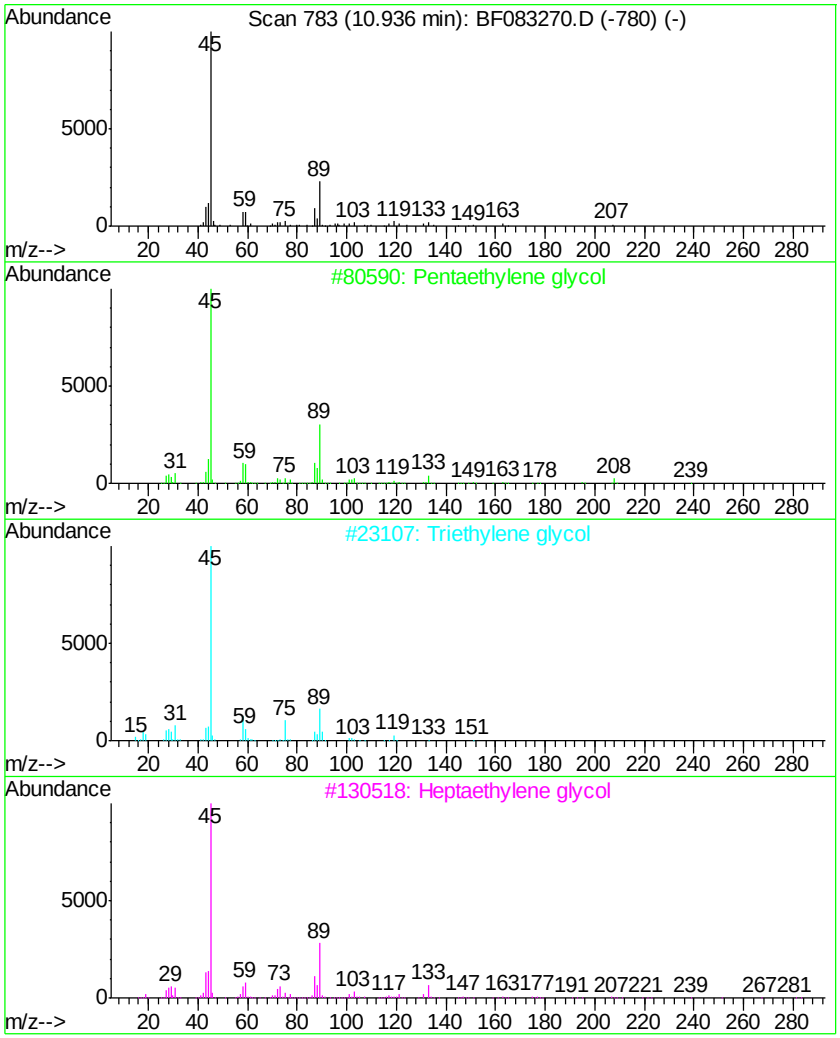
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

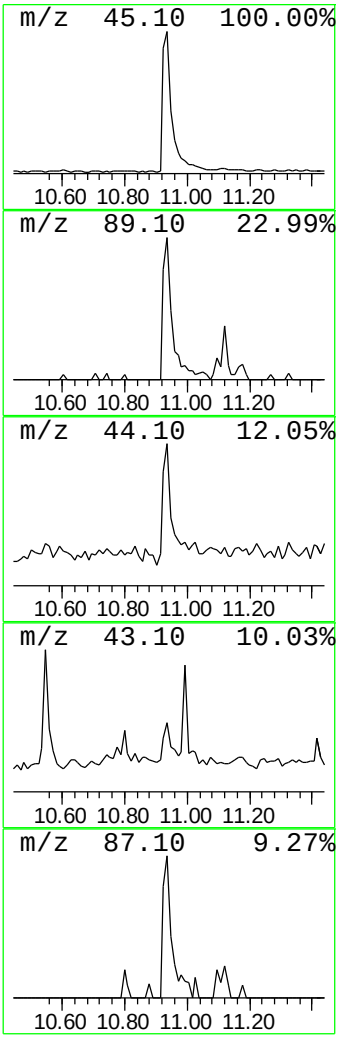
****

Peak Number 6 Pentaethylene glycol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.94	2.07 ng	167307	Phenanthrene-d10	11.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentaethylene glycol	238	C10H22O6	004792-15-8	90
2	Triethylene glycol	150	C6H14O4	000112-27-6	83
3	Heptaethylene glycol	326	C14H30O8	005617-32-3	74
4	Hexaqol	282	C12H26O7	002615-15-8	74
5	Ethanol, 2,2'-[oxybis(2,1-ethane...	194	C8H18O5	000112-60-7	64





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : MW-44

Quant Method : Z:\HPCHEM1\BNA_F\Methods\8270-BF112115.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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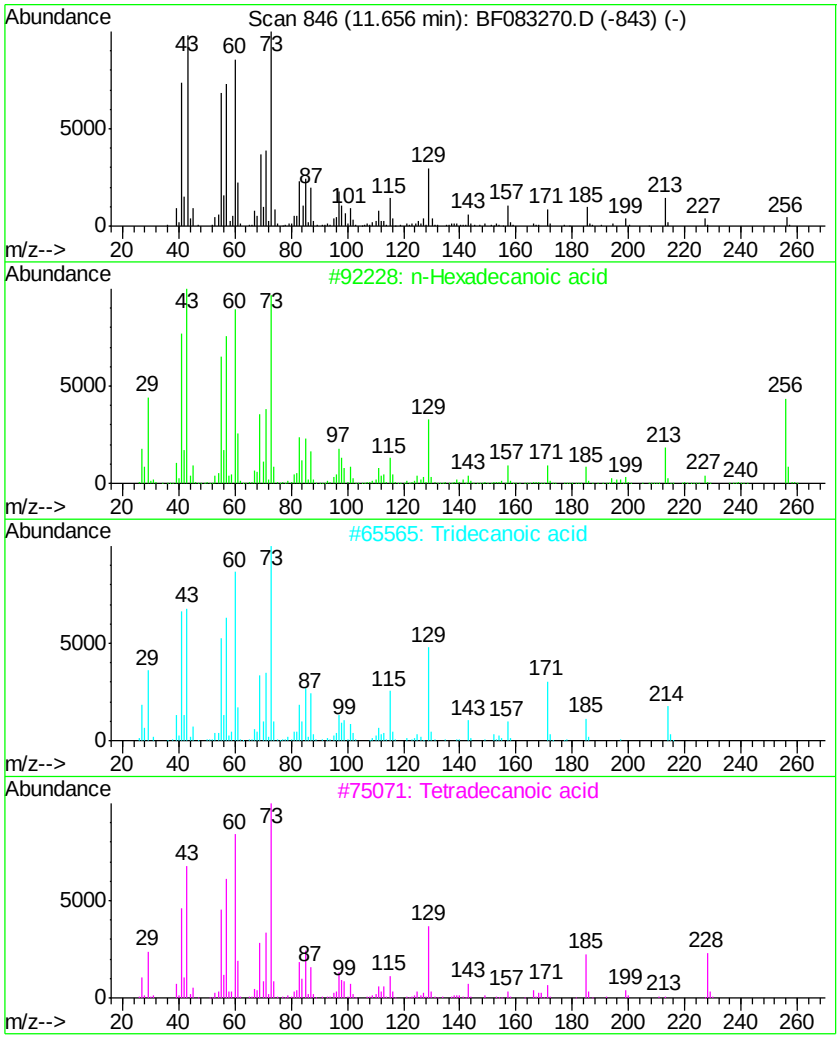
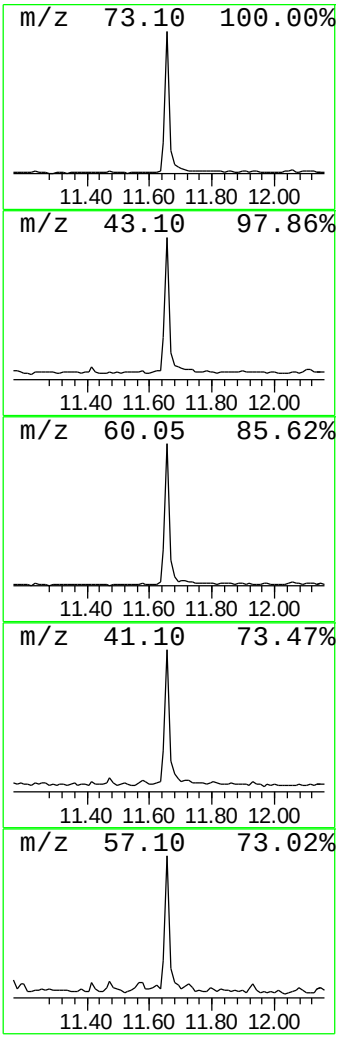
Peak Number 7 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	7.01 ng	568249	Phenanthrene-d10	11.10

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	96
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Nonanoic acid	158	C9H18O2	000112-05-0	11





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Operator : UM/IZ
Sample : G4534-02
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Instrument : BNA_F
ClientSampleId : MW-44

Quant Method : Z:\HPCHEM1\BNA_F\Methods\8270-BF112115.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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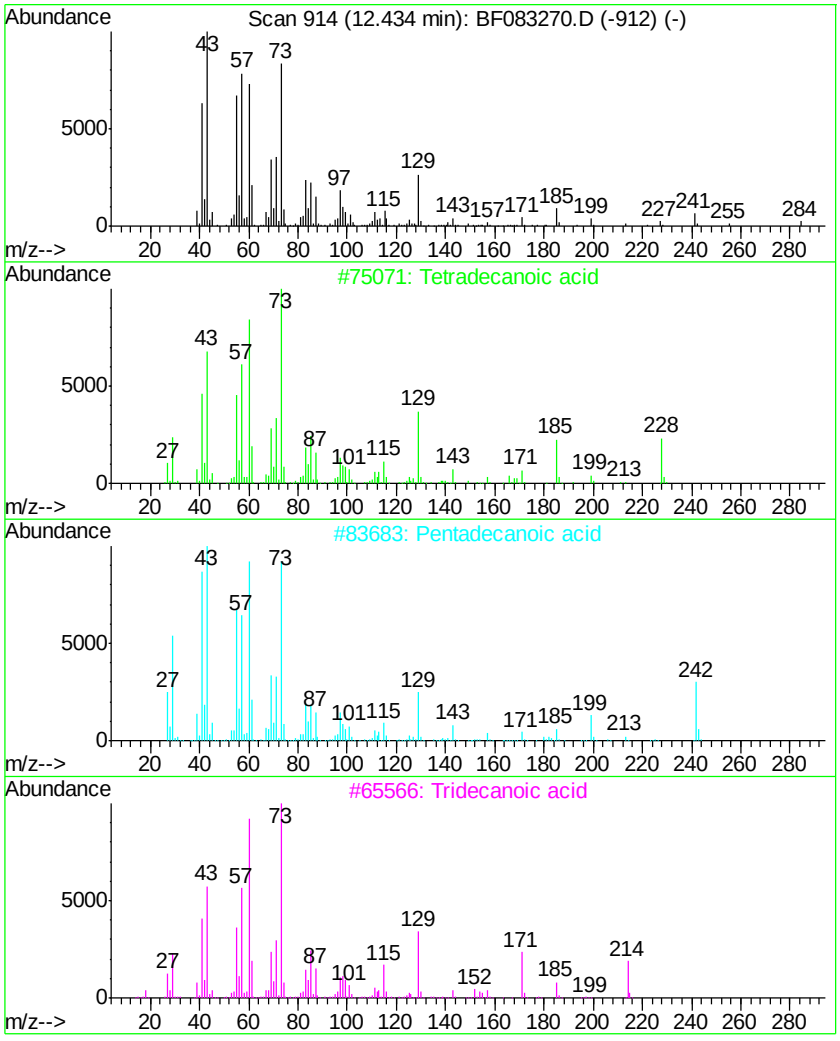
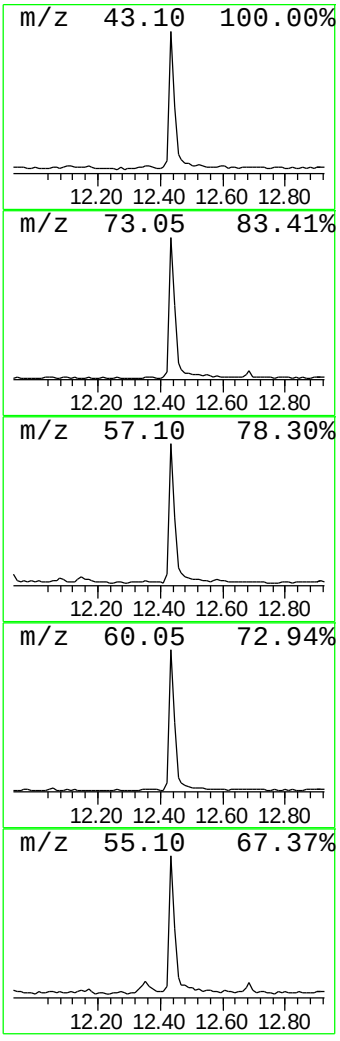
Peak Number 8 Tetradecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.43	11.09 ng	807699	Chrysene-d12	13.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	83
4	Undecanoic acid	186	C11H22O2	000112-37-8	72
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72





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Sample : G4534-02
Misc :
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Instrument : BNA_F
ClientSampleId : MW-44

Quant Method : Z:\HPCHEM1\BNA_F\Methods\8270-BF112115.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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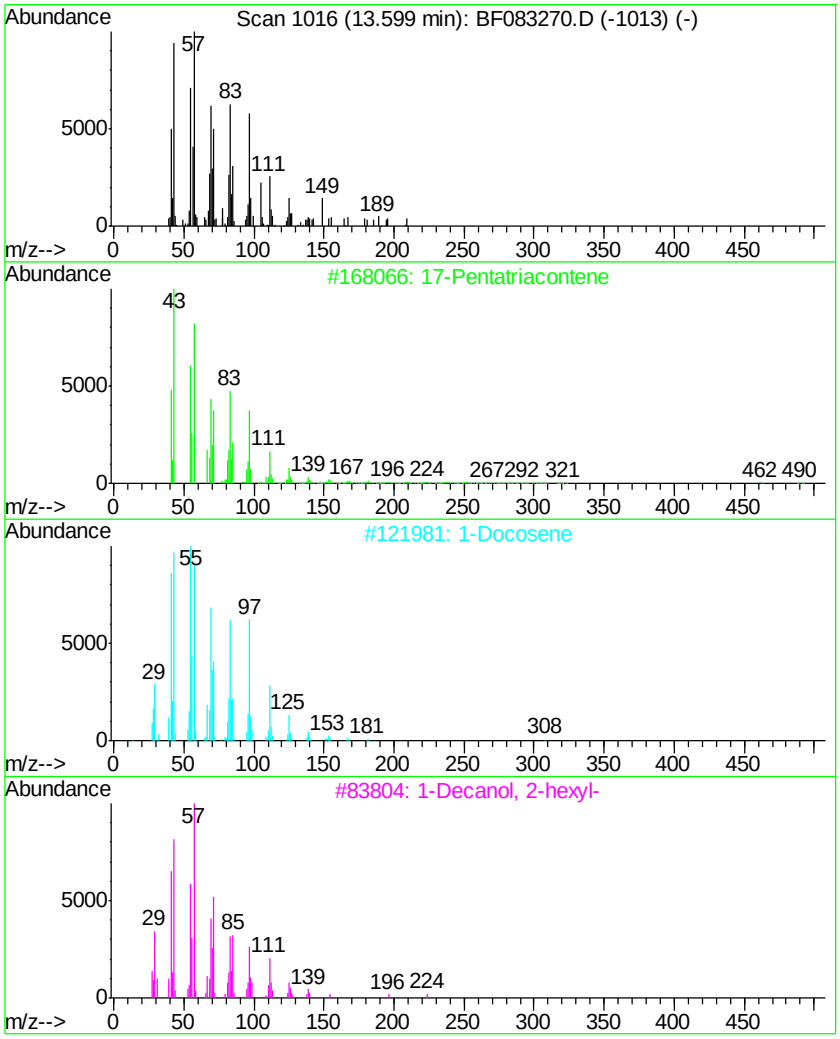
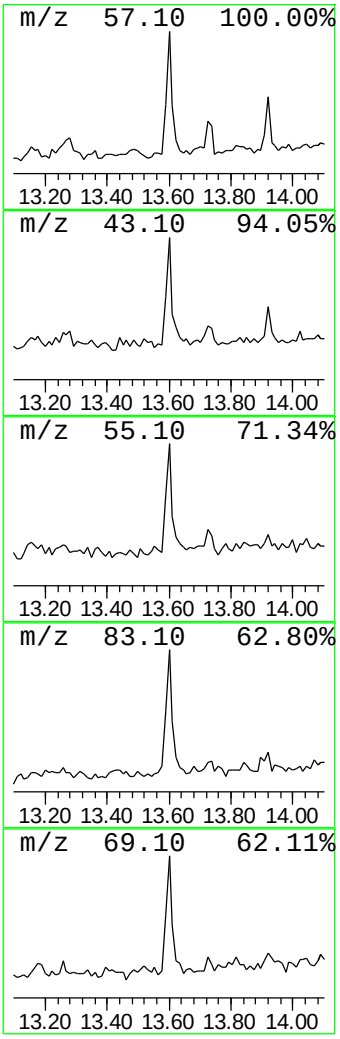
Peak Number 9 17-Pentatriacontene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.60	2.06 ng	149919	Chrysene-d12	13.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	83
2	1-Docosene	308	C22H44	001599-67-3	62
3	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	62
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	62
5	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112515\
Data File : BF083270.D
Acq On : 25 Nov 2015 13:29
Operator : UM/IZ
Sample : G4534-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-44

Quant Method : Z:\HPCHEM1\BNA_F\Methods\8270-BF112115.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
3-Penten-2-one, 4...	3.98	2.7	ng	135600	1	6.58	997076	20.0
2-Pentanone, 4-hy...	4.71	21.0	ng	1048360	1	6.58	997076	20.0
2-Pentanone, 4-me...	5.59	2.5	ng	124704	1	6.58	997076	20.0
unknown6.36	6.36	59.4	ng	2958700	1	6.58	997076	20.0
Pentaethylene glycol	10.94	2.1	ng	167307	4	11.10	1620350	20.0
n-Hexadecanoic acid	11.66	7.0	ng	568249	4	11.10	1620350	20.0
Tetradecanoic acid	12.43	11.1	ng	807699	5	13.73	1456330	20.0
17-Pentatriacontene	13.60	2.1	ng	149919	5	13.73	1456330	20.0