LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083763.D
Acq On : 14 Dec 2015 7:25
Operator : UM/IZ
Sample : G4648-10
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04(0-0.16)

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-BF121315.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	2.224	9	12	14	rBV	24455	37124	1.30%	0.147%
2	5.116	262	265	269	rBV	445081	608330	21.23%	2.407%
3	5.527	298	301	304	rBV	2435903	2557235	89.23%	10.119%
4	6.544	387	390	393	rBV	2127226	2387010	83.29%	9.446%
5	6.693	400	403	405	rBV	2118705	2865731	100.00%	11.340%
6	6.922	420	423	425	rVB	692472	619042	21.60%	2.450%
7	7.082	434	437	439	rVB	2206935	2388018	83.33%	9.450%
8	7.482	469	472	474	rBV	1682939	1827497	63.77%	7.232%
9	8.202	533	535	537	rBV	884500	723425	25.24%	2.863%
10	9.276	626	629	632	rBV	2814039	2795830	97.56%	11.063%
11	9.665	661	663	666	rBV	373022	359620	12.55%	1.423%
12	9.893	681	683	686	rBV	41710	34277	1.20%	0.136%
13	9.950	686	688	691	rVB	570122	651308	22.73%	2.577%
14	10.396	723	727	728	rBV	48595	57964	2.02%	0.229%
15	10.739	754	757	759	rBV	1548472	1450379	50.61%	5.739%
16	10.865	766	768	773	rBV	56716	57087	1.99%	0.226%
17	11.436	816	818	820	rBV	683381	623360	21.75%	2.467%
18	12.842	939	941	944	rBV	171342	161816	5.65%	0.640%
19	12.922	944	948	950	rVB	57329	59507	2.08%	0.235%
20	13.014	954	956	959	rBV	2261969	2537194	88.54%	10.040%
21	13.551	1001	1003	1005	rBV	140693	134192	4.68%	0.531%
22	13.597	1005	1007	1011	rVB2	38563	55542	1.94%	0.220%
23	13.917	1032	1035	1045	rBV	170988	295875	10.32%	1.171%
24	14.065	1045	1048	1050	rBV	590902	701905	24.49%	2.777%
25	14.237	1061	1063	1069	rBV	66107	71730	2.50%	0.284%
26	14.545	1088	1090	1092	rBV	88686	96395	3.36%	0.381%
27	14.842	1114	1116	1120	rBV	52307	63074	2.20%	0.250%
28	15.174	1143	1145	1150	rVB2	39886	59670	2.08%	0.236%
29	15.505	1171	1174	1176	rBV	411662	559832	19.54%	2.215%
30	15.551	1176	1178	1182	rVB	37191	59141	2.06%	0.234%
31	15.985	1213	1216	1218	rBV	27504	47640	1.66%	0.189%
32	16.477	1254	1259	1262	rBV2	26960	67891	2.37%	0.269%
33	17.060	1307	1310	1315	rBV	26011	56170	1.96%	0.222%
34	17.757	1367	1371	1384	rVB	30530	119407	4.17%	0.473%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083763.D
Acq On : 14 Dec 2015 7:25
Operator : UM/IZ
Sample : G4648-10
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04(0-0.16)

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-BF121315.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	18.568	1438	1442	1449	rBV2	24265	81027	2.83%	0.321%

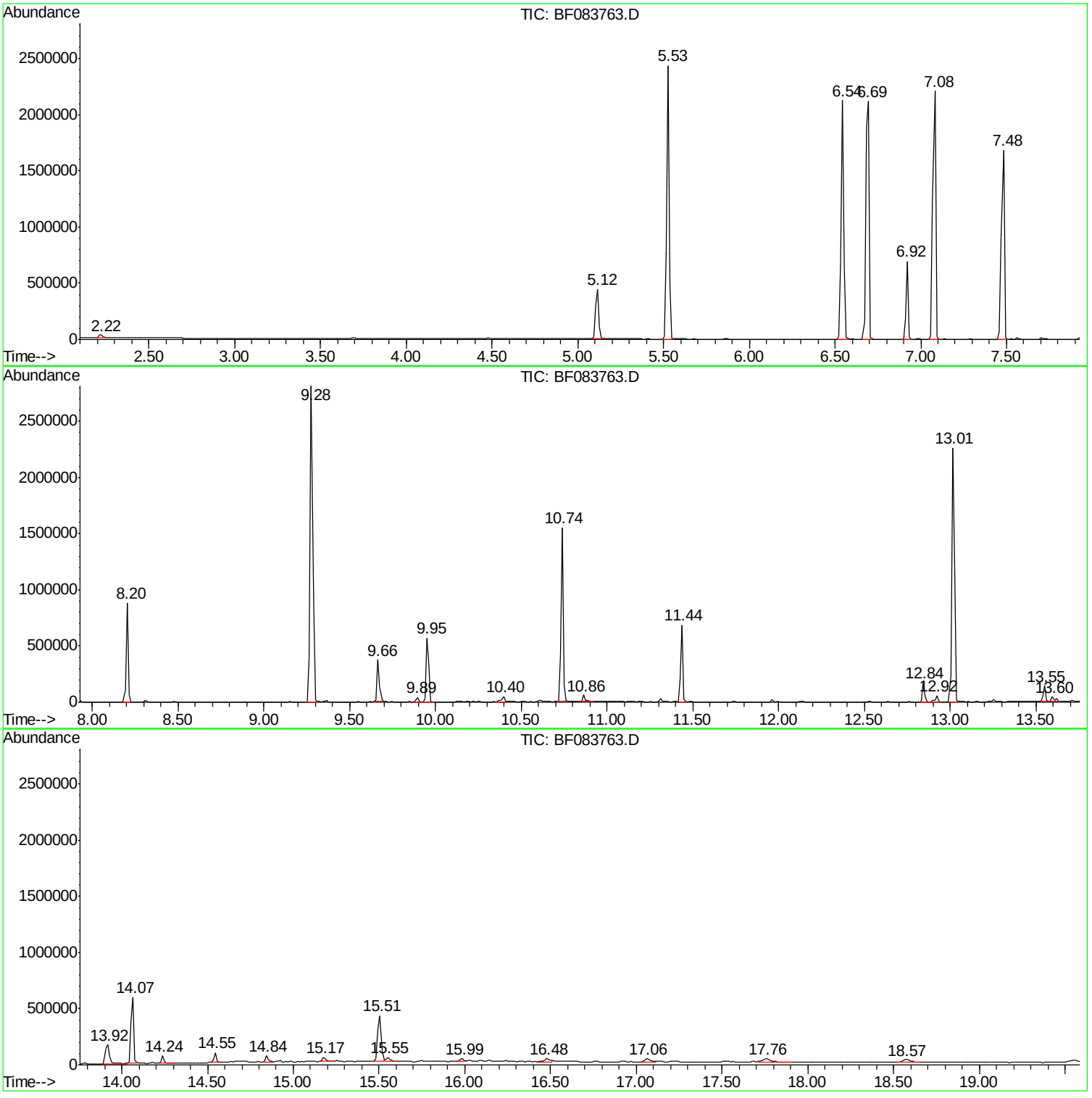
Sum of corrected areas: 25271245

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083763.D
Acq On : 14 Dec 2015 7:25
Operator : UM/IZ
Sample : G4648-10
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.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\BF121315\
Data File : BF083763.D
Acq On : 14 Dec 2015 7:25
Operator : UM/IZ
Sample : G4648-10
Misc :
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Instrument : BNA_F
ClientSampleId : SB-04(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

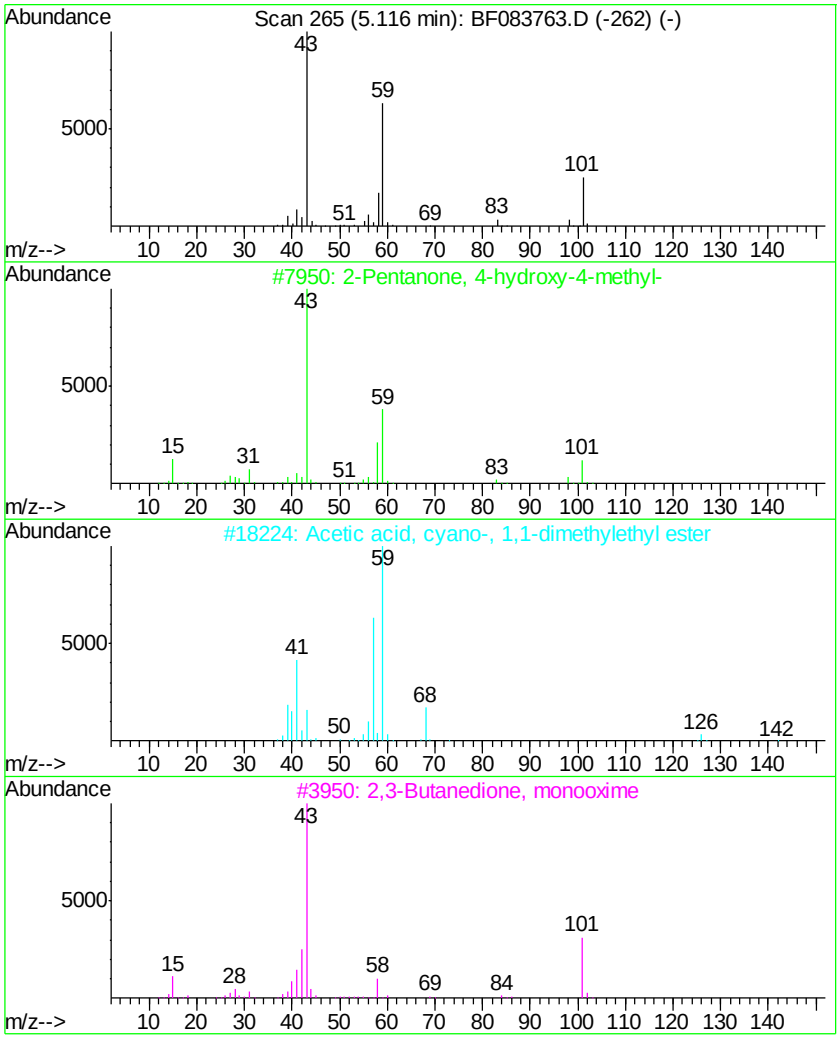
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

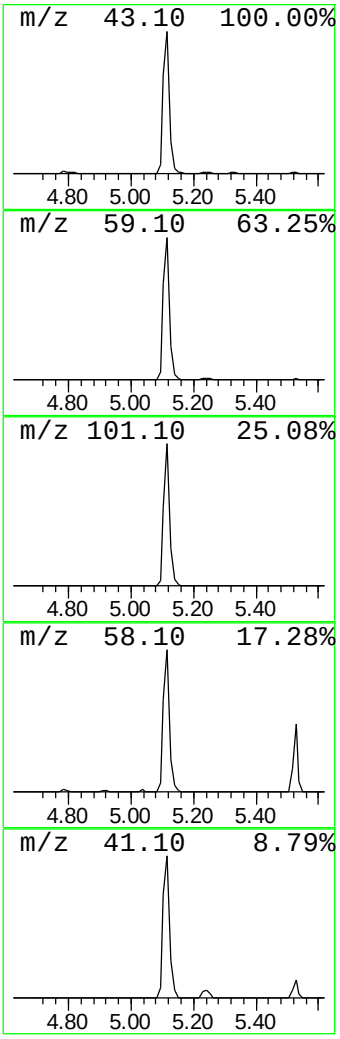
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	19.65 ng	608330	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
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\BF121315\
Data File : BF083763.D
Acq On : 14 Dec 2015 7:25
Operator : UM/IZ
Sample : G4648-10
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

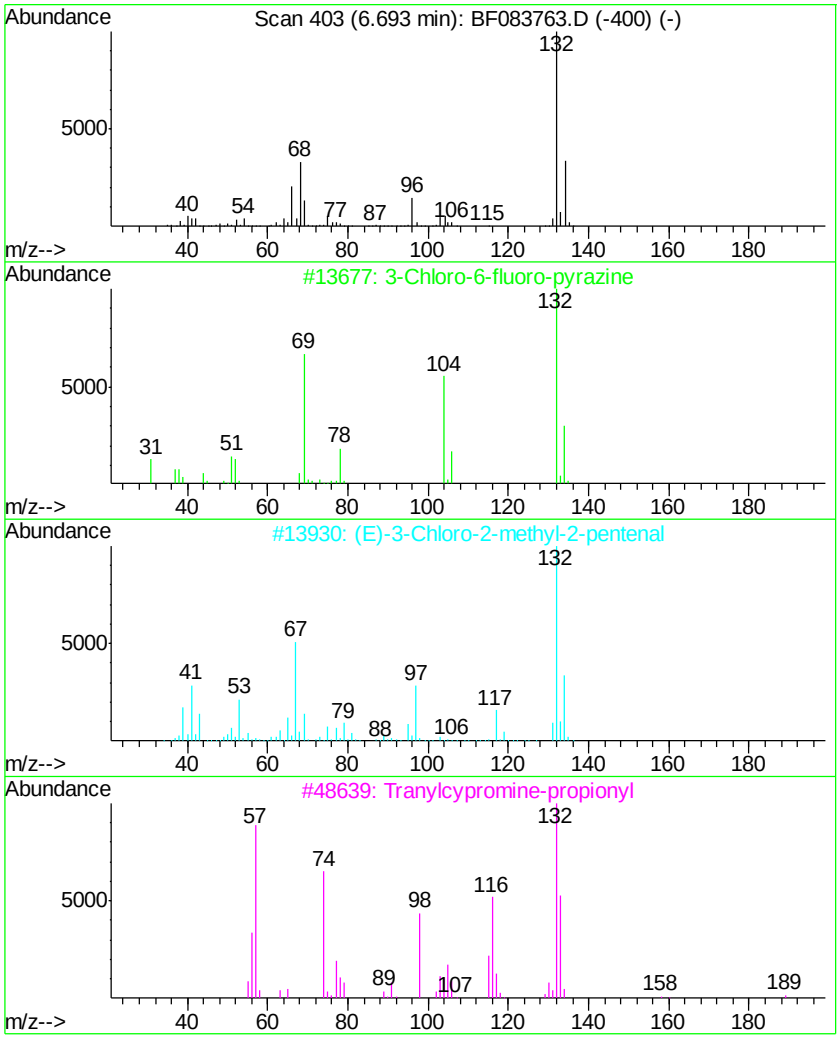
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

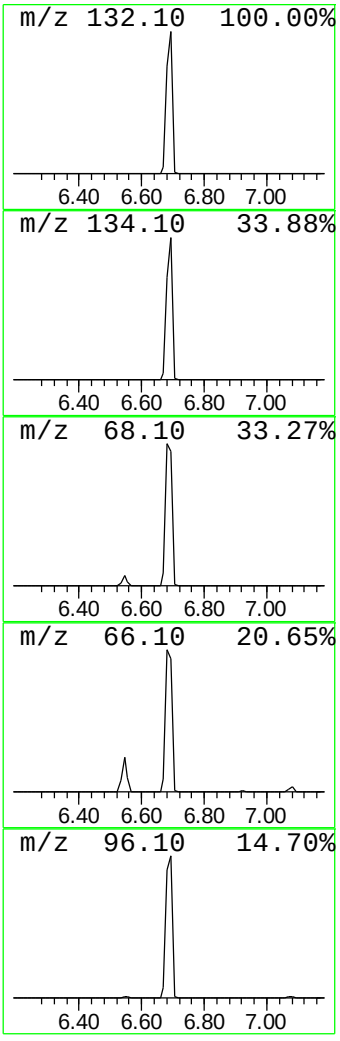
****

Peak Number 2 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	92.59 ng	2865730	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
5	Xenon	132	Xe	007440-63-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083763.D
Acq On : 14 Dec 2015 7:25
Operator : UM/IZ
Sample : G4648-10
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

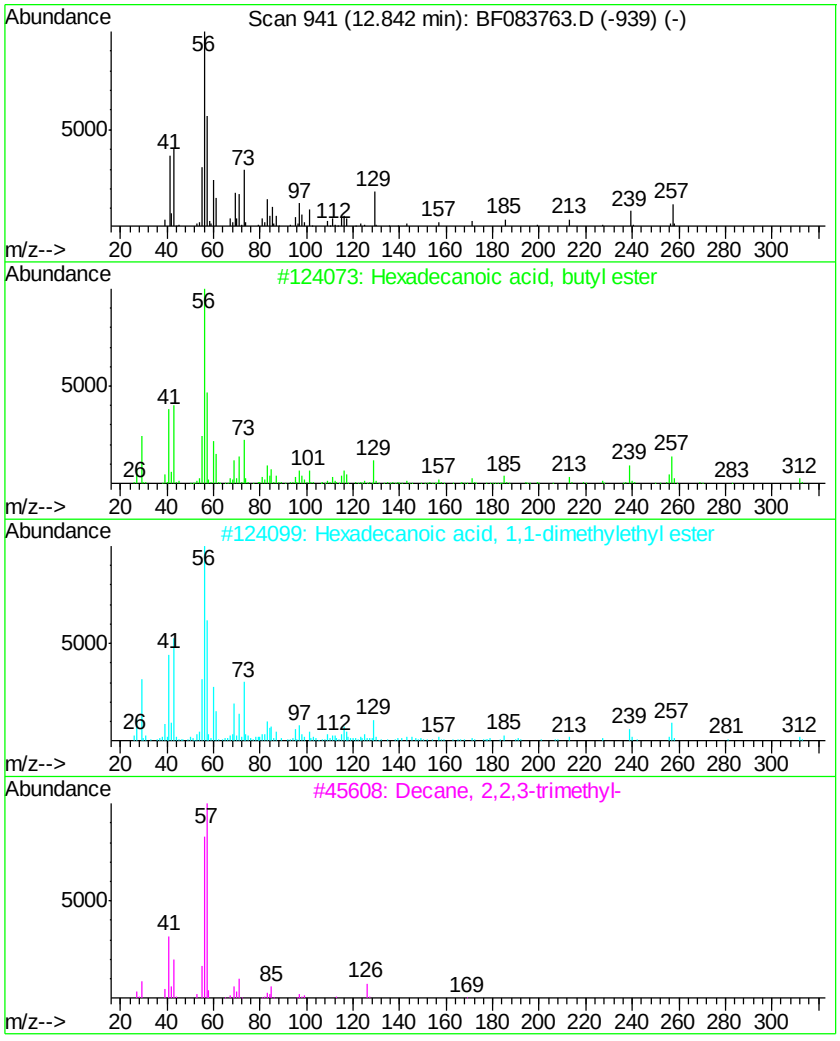
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

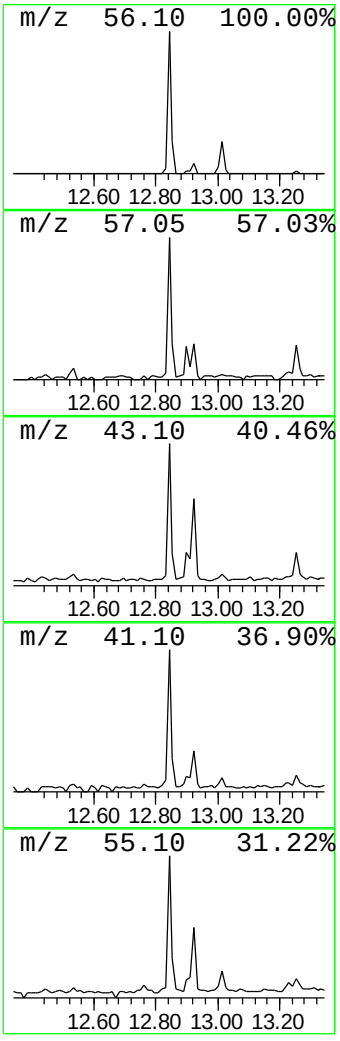
****

Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	4.61 ng	161816	Chrysene-d12	14.07

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	91
3	Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	38
4	Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	38
5	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083763.D
Acq On : 14 Dec 2015 7:25
Operator : UM/IZ
Sample : G4648-10
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

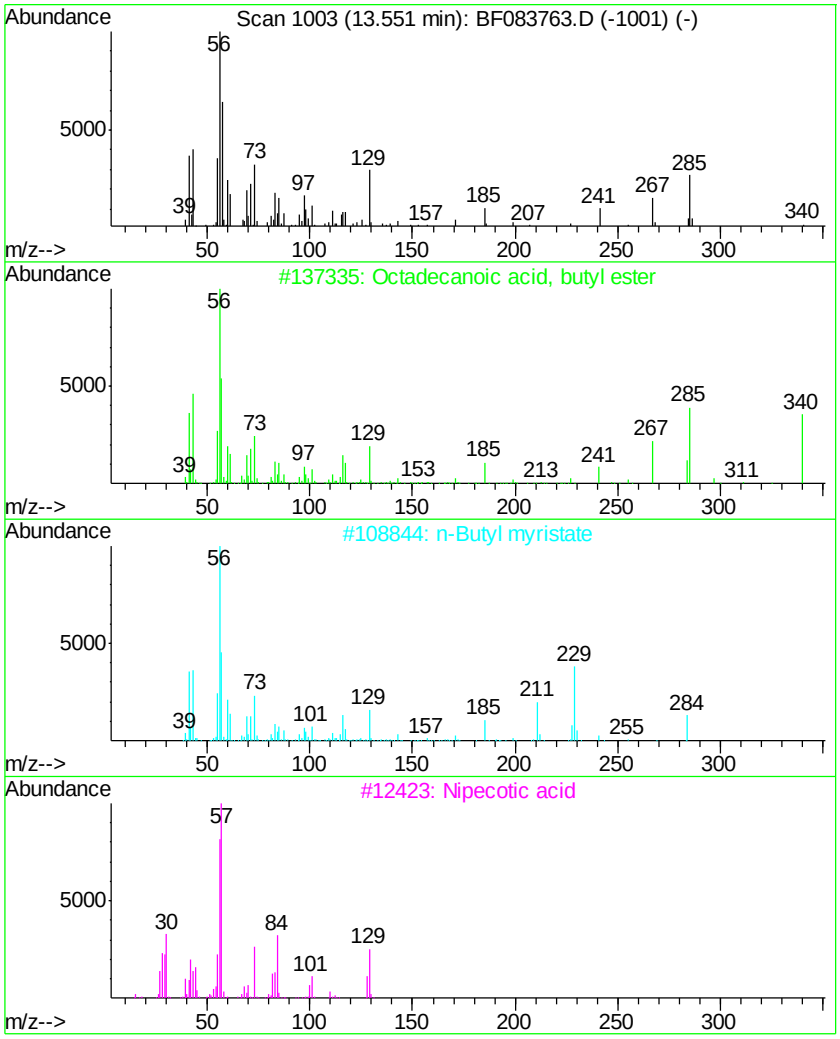
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

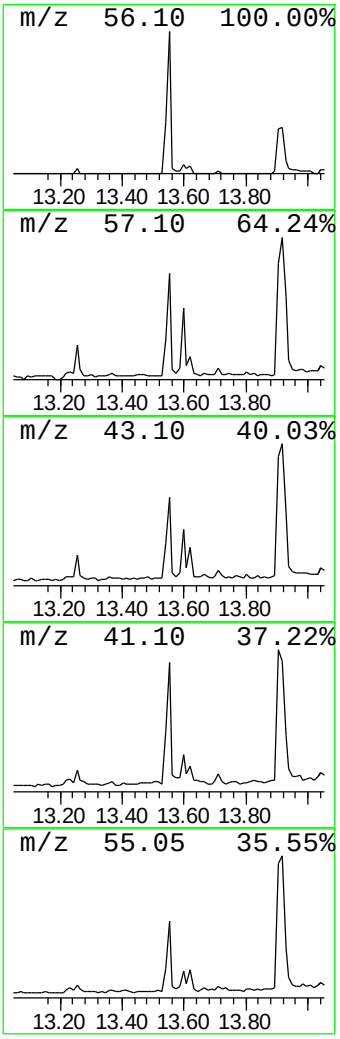
****

Peak Number 5 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	3.82 ng	134192	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	93
2	n-Butyl myristate	284	C18H36O2	000110-36-1	50
3	Nipecotic acid	129	C6H11NO2	000498-95-3	47
4	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	42
5	2-Methyl-1-octadecene	266	C19H38	061868-20-0	27





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Data File : BF083763.D
Acq On : 14 Dec 2015 7:25
Operator : UM/IZ
Sample : G4648-10
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

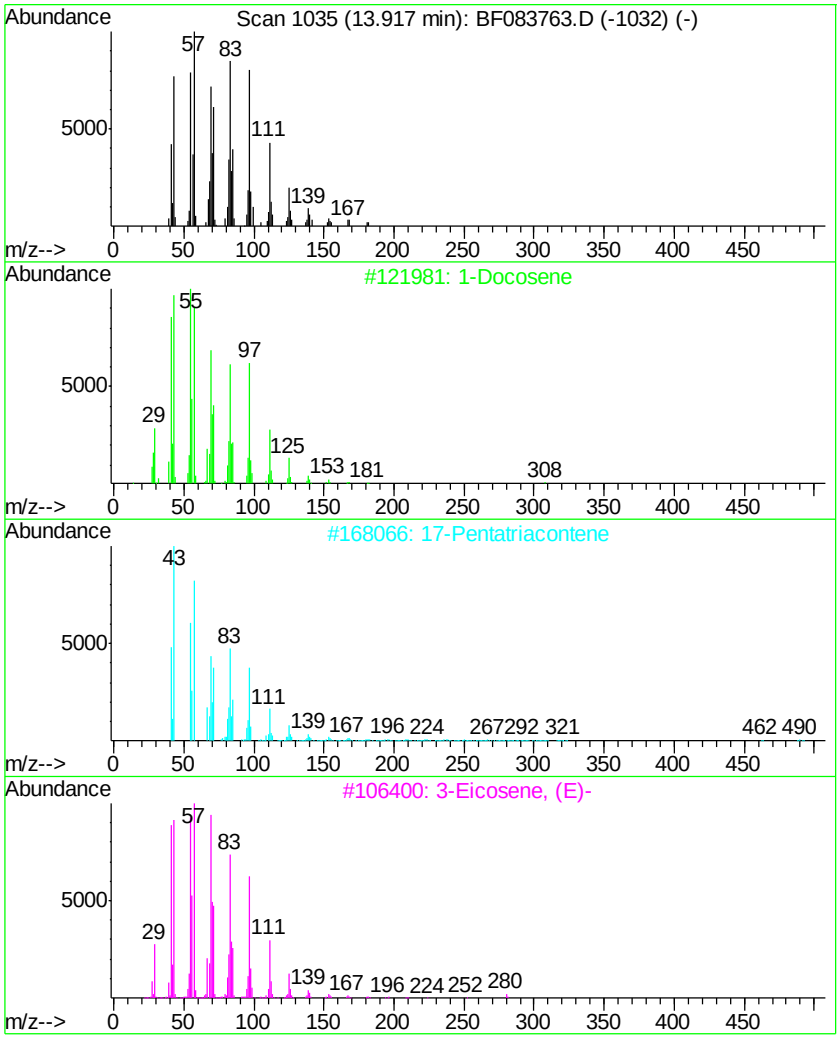
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

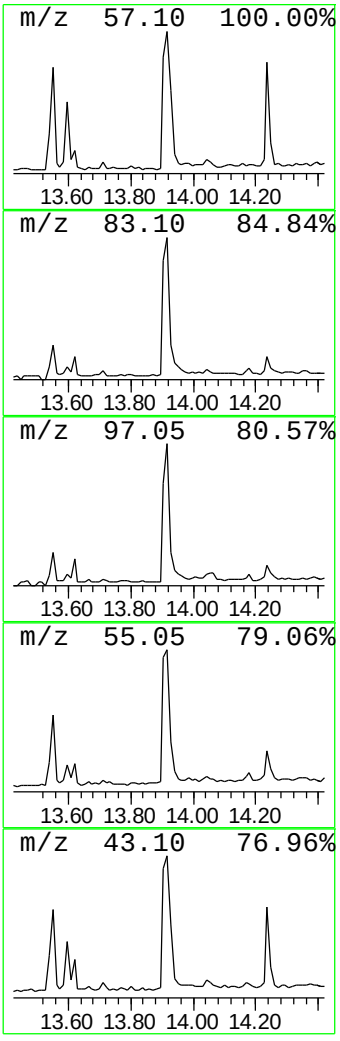
****

Peak Number 6 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	8.43 ng	295875	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	91
2	17-Pentatriacontene	491	C35H70	006971-40-0	91
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	87
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
5	1-Tetracosanol	354	C24H50O	000506-51-4	83





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Data File : BF083763.D
Acq On : 14 Dec 2015 7:25
Operator : UM/IZ
Sample : G4648-10
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.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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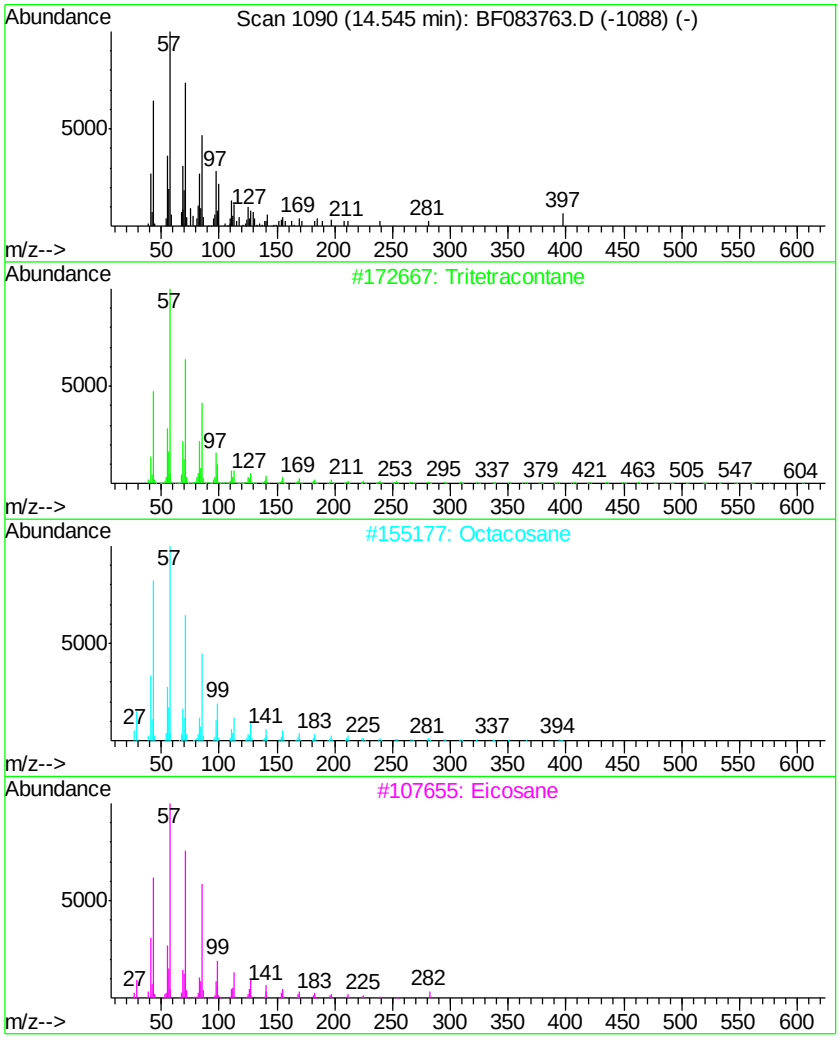
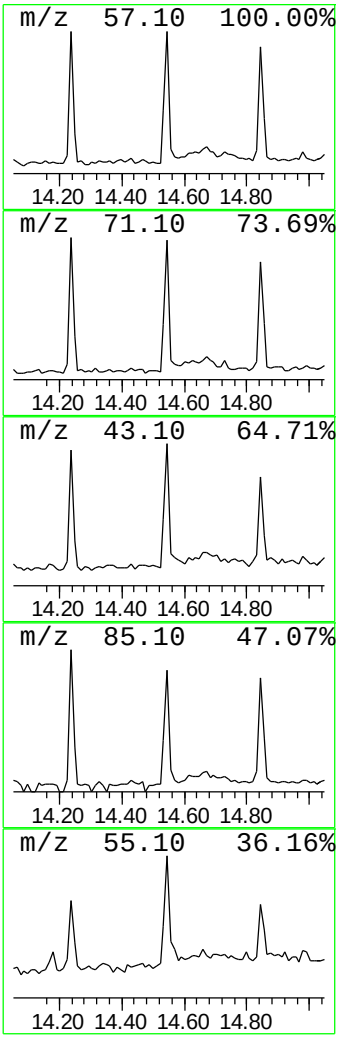
Peak Number 7 Tritetracontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.55	2.75 ng	96395	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tritetracontane	605	C43H88	007098-21-7	83
2	Octacosane	394	C28H58	000630-02-4	72
3	Eicosane	282	C20H42	000112-95-8	68
4	Heneicosane	296	C21H44	000629-94-7	64
5	Triacontane	422	C30H62	000638-68-6	64





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Data File : BF083763.D
Acq On : 14 Dec 2015 7:25
Operator : UM/IZ
Sample : G4648-10
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.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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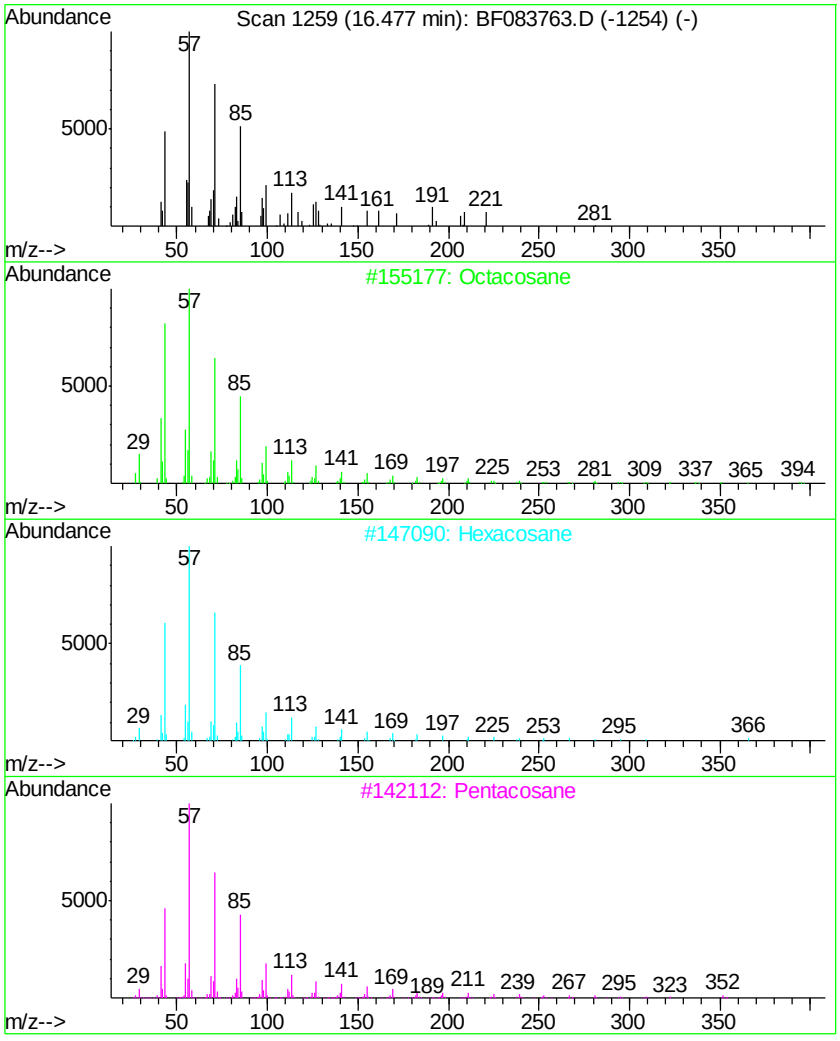
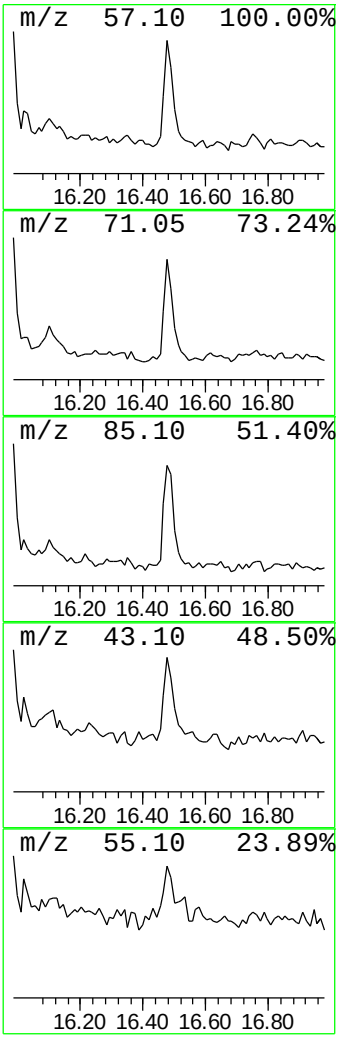
Peak Number 8 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.48	2.43 ng	67891	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	87
2	Hexacosane	366	C26H54	000630-01-3	86
3	Pentacosane	352	C25H52	000629-99-2	80
4	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	80
5	Heneicosane	296	C21H44	000629-94-7	78





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083763.D
Acq On : 14 Dec 2015 7:25
Operator : UM/IZ
Sample : G4648-10
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.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...	5.12	19.6	ng	608330	1	6.92	619042	20.0
unknown6.69	6.69	92.6	ng	2865730	1	6.92	619042	20.0
Hexadecanoic acid...	12.84	4.6	ng	161816	5	14.07	701905	20.0
Octadecanoic acid...	13.55	3.8	ng	134192	5	14.07	701905	20.0
1-Docosene	13.92	8.4	ng	295875	5	14.07	701905	20.0
Tritetracontane	14.55	2.8	ng	96395	5	14.07	701905	20.0
Octacosane	16.48	2.4	ng	67891	6	15.51	559832	20.0