LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081476.D
Acq On : 5 Sep 2015 21:28
Operator : UM/IZ
Sample : G3555-01
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1

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-BF090115.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	4.398	243	246	262	rVB	503094	948077	53.56%	6.073%
2	4.901	288	290	293	rBV	1285622	1590048	89.82%	10.185%
3	6.021	385	388	391	rBV	1245983	1699505	96.00%	10.886%
4	6.124	395	397	399	rBV	1857234	1662700	93.92%	10.651%
5	6.353	415	417	420	rVB	398360	349746	19.76%	2.240%
6	6.513	429	431	433	rBV	1426822	1272838	71.90%	8.153%
7	6.936	465	468	470	rBV	1128105	1136043	64.17%	7.277%
8	7.645	528	530	532	rBV	560419	461849	26.09%	2.958%
9	8.730	622	625	627	rBV	1881528	1770264	100.00%	11.340%
10	9.130	658	660	663	rBV	336230	276831	15.64%	1.773%
11	9.382	680	682	685	rVB	484393	451974	25.53%	2.895%
12	10.170	748	751	753	rBV	1001180	1026920	58.01%	6.578%
13	10.319	762	764	767	rBV	26461	27959	1.58%	0.179%
14	10.765	801	803	804	rBV	22681	18698	1.06%	0.120%
15	10.845	808	810	813	rBV	467367	440696	24.89%	2.823%
16	11.428	859	861	866	rBV	45083	63317	3.58%	0.406%
17	12.285	934	936	939	rBV	63923	89844	5.08%	0.576%
18	12.342	939	941	942	rBV	15200	21110	1.19%	0.135%
19	12.365	942	943	946	rVB	22748	21384	1.21%	0.137%
20	12.434	946	949	951	rBV	1547627	1397945	78.97%	8.955%
21	12.994	996	998	1000	rBV	68174	67579	3.82%	0.433%
22	13.359	1028	1030	1036	rBV	60341	132070	7.46%	0.846%
23	13.451	1036	1038	1041	rVV	351161	328454	18.55%	2.104%
24	13.679	1055	1058	1060	rBV	24156	24502	1.38%	0.157%
25	13.977	1082	1084	1086	rBV	29062	28219	1.59%	0.181%
26	14.274	1108	1110	1112	rBV	19508	20349	1.15%	0.130%
27	14.548	1132	1134	1137	rBV	24918	28613	1.62%	0.183%
28	14.765	1150	1153	1155	rBV	194020	233256	13.18%	1.494%
29	15.154	1184	1187	1190	rBV	15885	20515	1.16%	0.131%

Sum of corrected areas: 15611305

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Misc :
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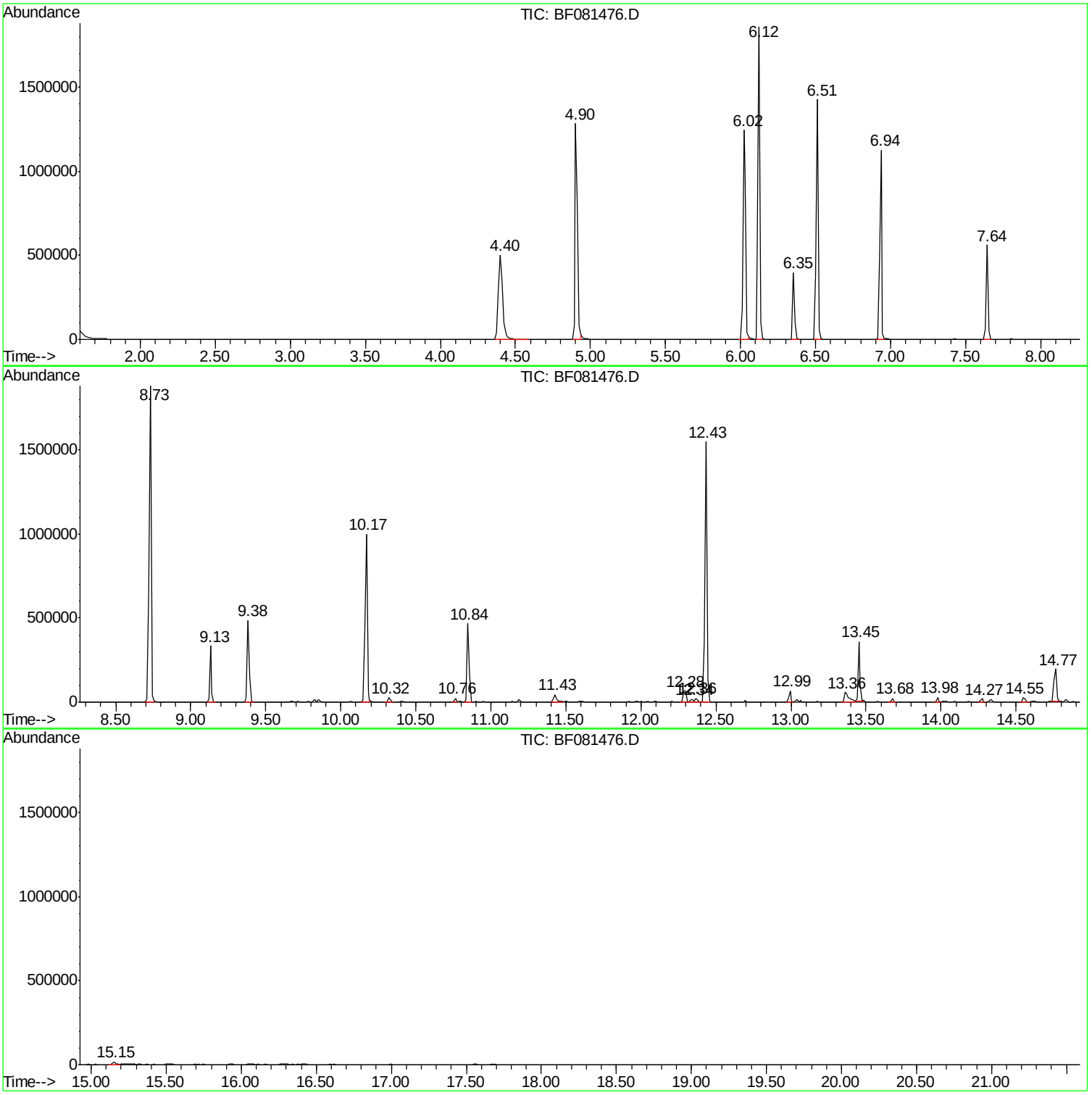
Instrument : BNA_F
ClientSampleId : SB-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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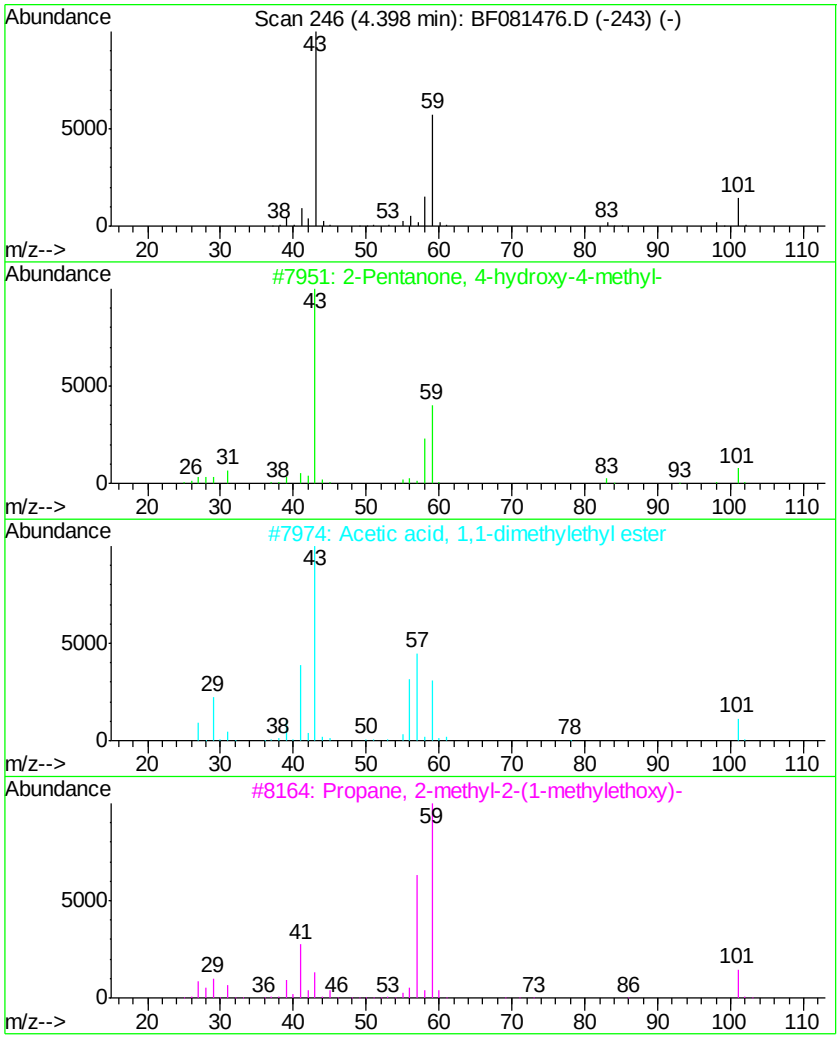
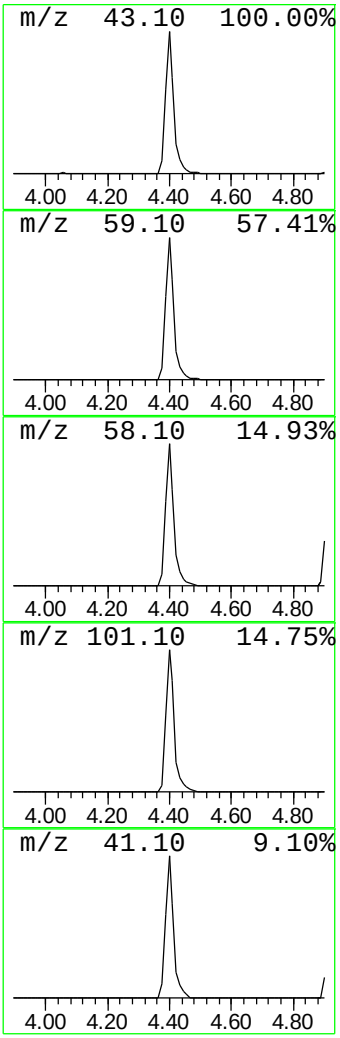
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	54.22 ng	948077	1,4-Dichlorobenzene-d4	6.35

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	38
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33





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Operator : UM/IZ
Sample : G3555-01
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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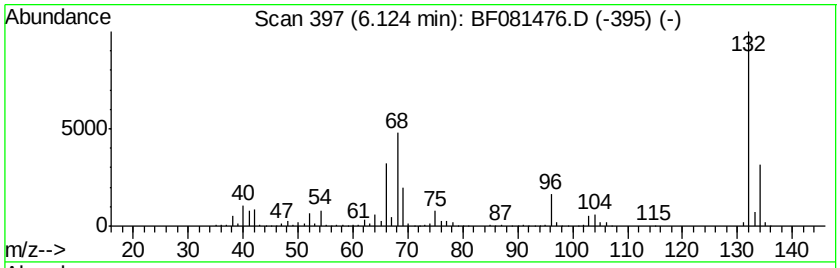
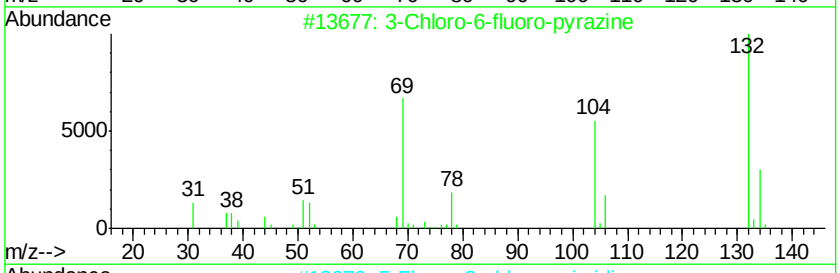
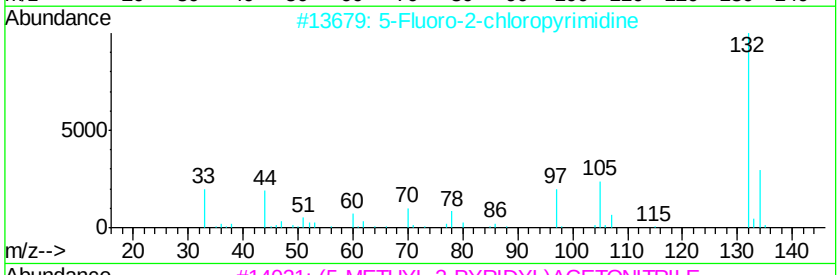
Peak Number 2 unknown6.12 Concentration Rank 1

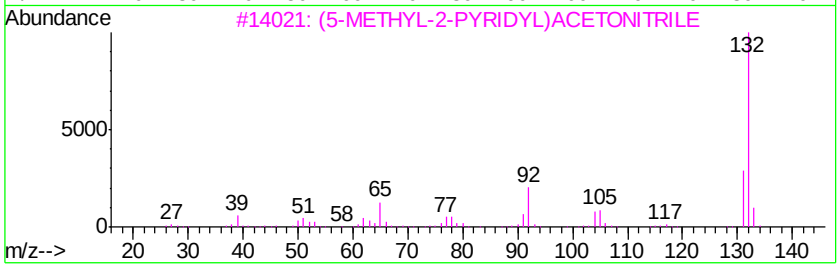
R.T.	EstConc	Area	Relative to ISTD	R.T.
6.12	95.08 ng	1662700	1,4-Dichlorobenzene-d4	6.35

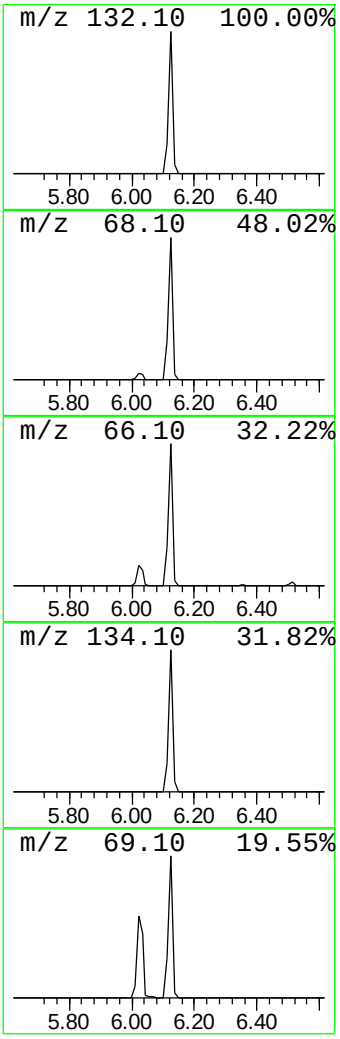
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Xenon	132	Xe	007440-63-3	9











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Sample : G3555-01
Misc :
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Instrument : BNA_F
ClientSampleId : SB-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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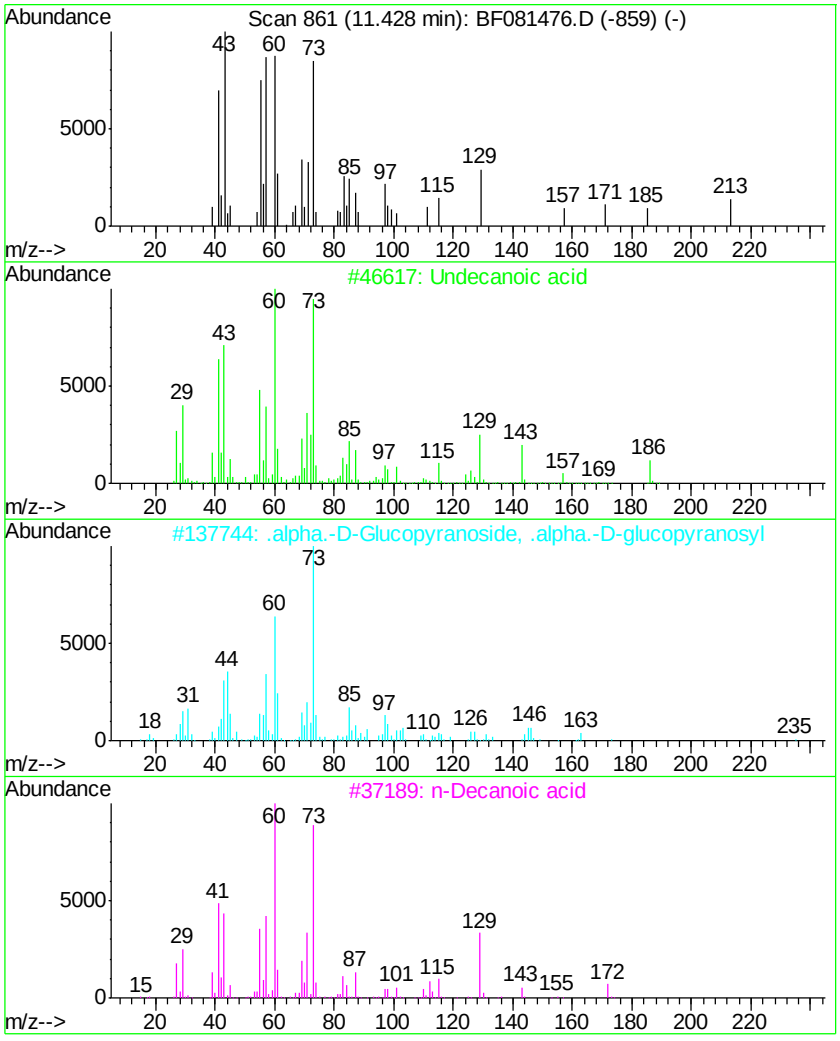
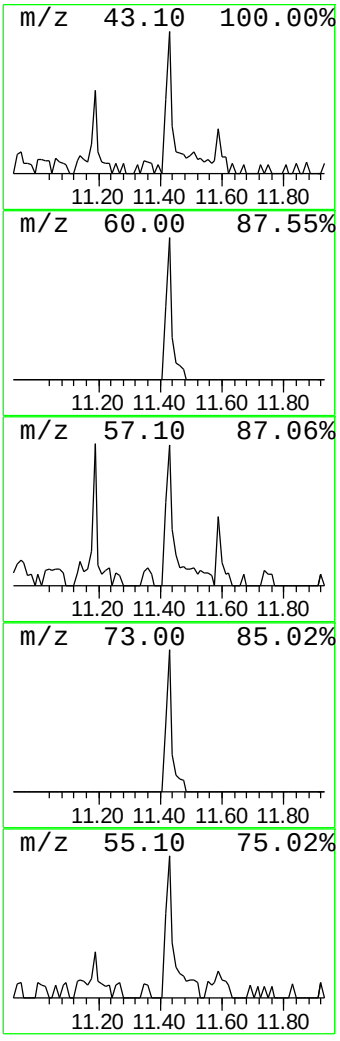
Peak Number 4 Undecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	2.87 ng	63317	Phenanthrene-d10	10.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	59
2	.alpha.-D-Glucopyranoside, .alph...	342	C12H22O11	000099-20-7	47
3	n-Decanoic acid	172	C10H20O2	000334-48-5	47
4	Nonanoic acid	158	C9H18O2	000112-05-0	43
5	Lactose	342	C12H22O11	000063-42-3	40





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Data File : BF081476.D
Acq On : 5 Sep 2015 21:28
Operator : UM/IZ
Sample : G3555-01
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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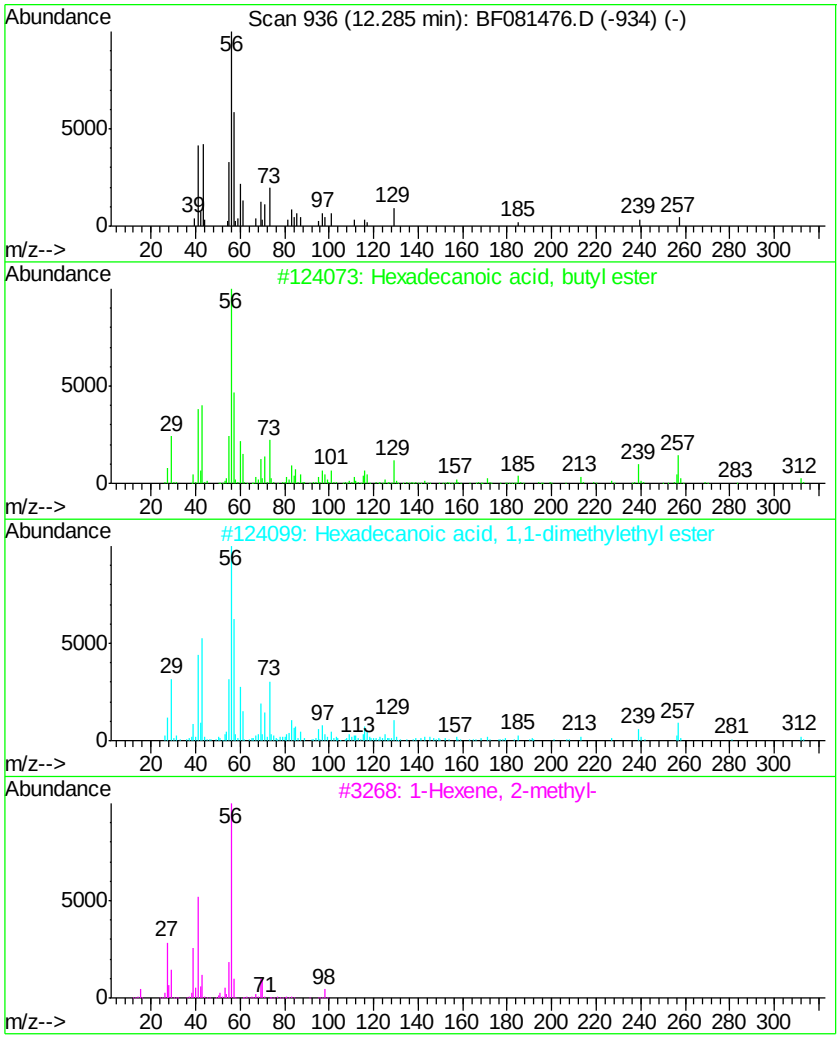
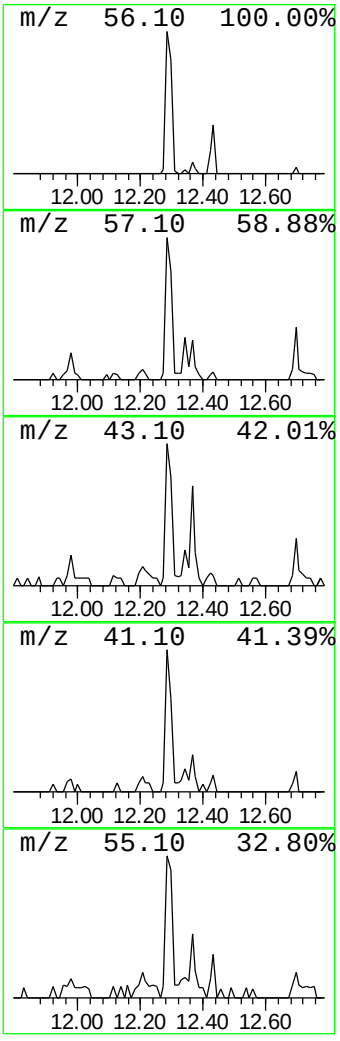
Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	5.47 ng	89844	Chrysene-d12	13.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	78
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	78
3	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	38
4	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	37
5	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	37





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081476.D
Acq On : 5 Sep 2015 21:28
Operator : UM/IZ
Sample : G3555-01
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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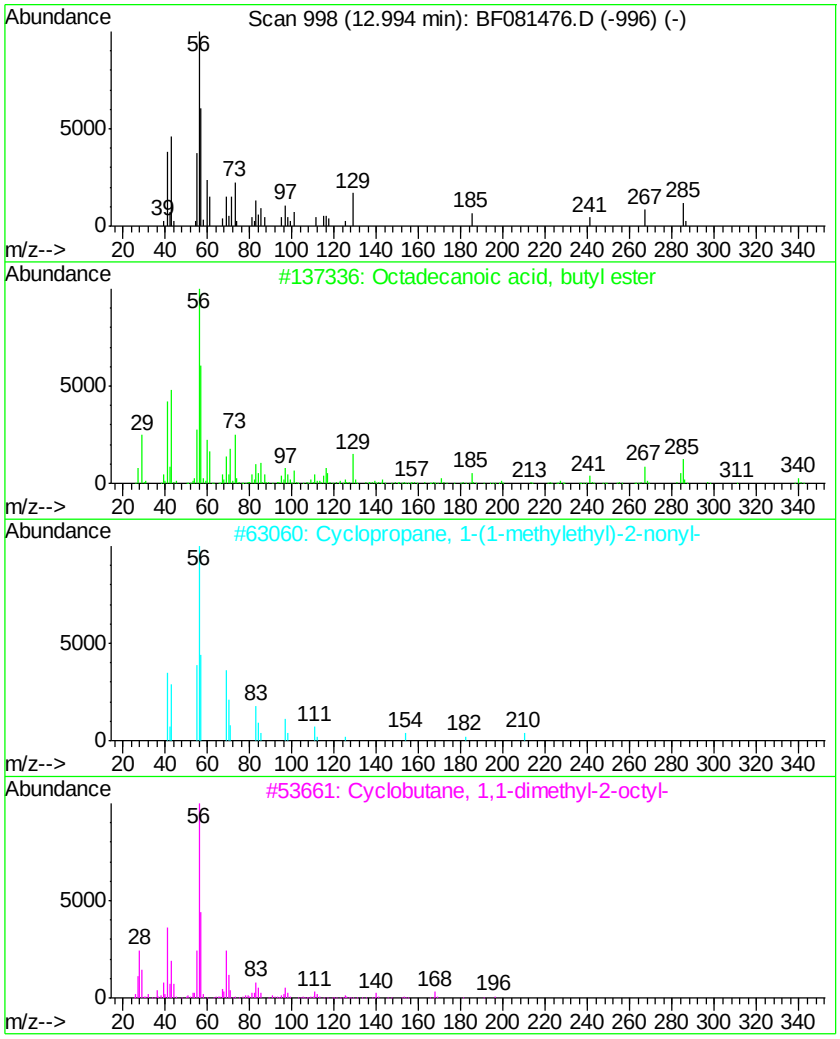
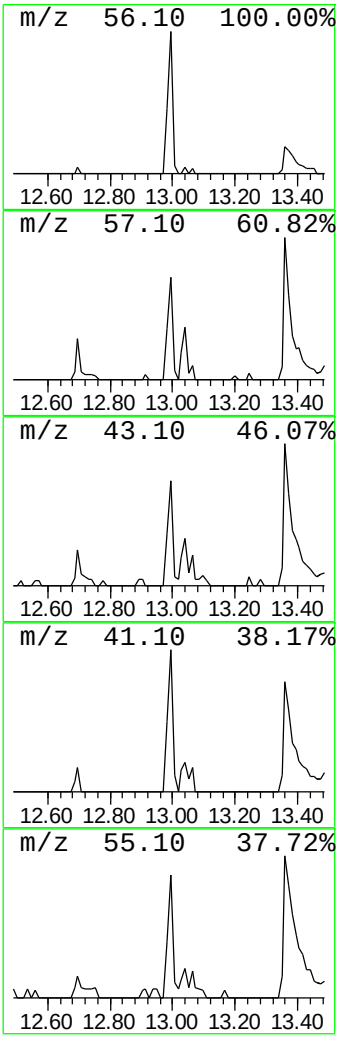
Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.99	4.11 ng	67579	Chrysene-d12	13.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	58
2	Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	38
3	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
4	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37
5	1-Pentadecene, 2-methyl-	224	C16H32	029833-69-0	37





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Sample : G3555-01
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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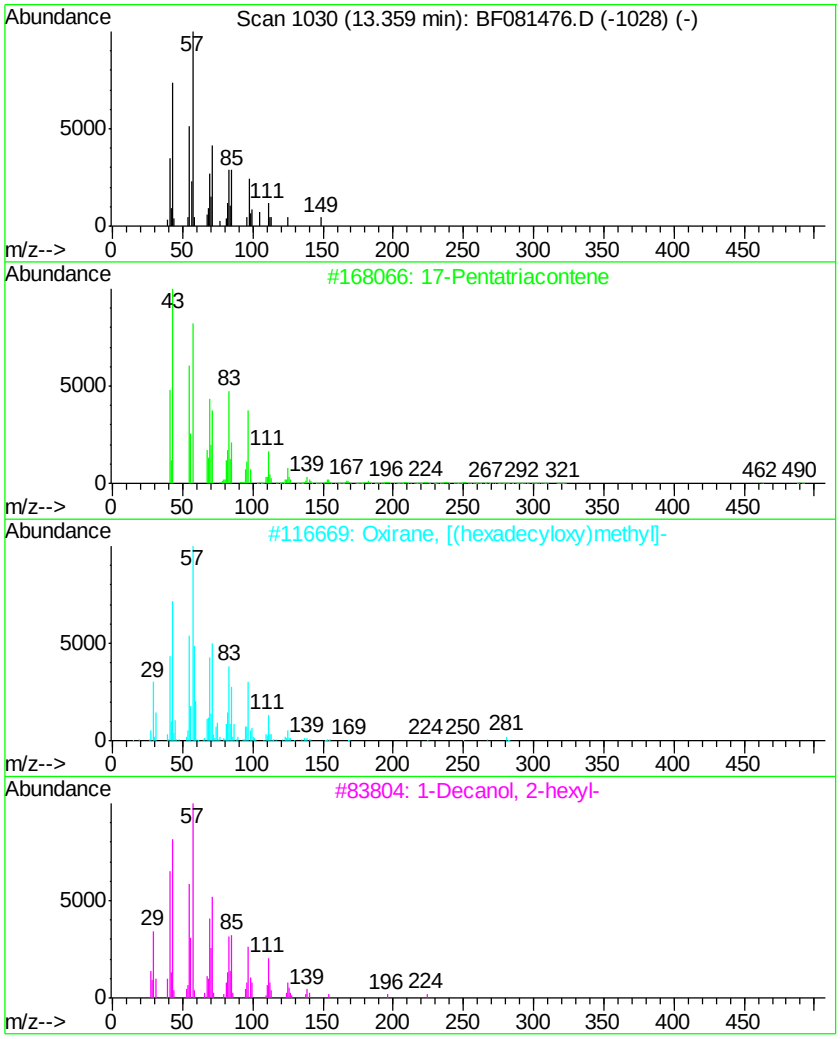
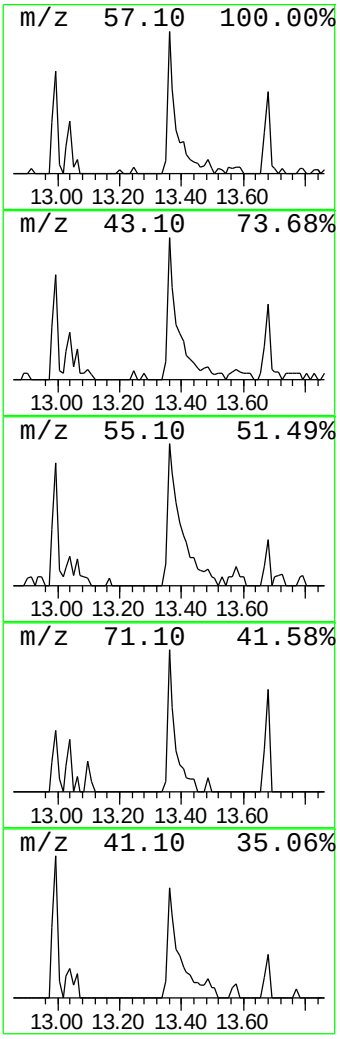
Peak Number 7 17-Pentatriacontene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.36	8.04 ng	132070	Chrysene-d12	13.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	58
2	Oxirane, [(hexadecyloxy)methyl]-	298	C19H38O2	015965-99-8	58
3	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	58
4	2-Hexyl-1-octanol	214	C14H30O	019780-79-1	53
5	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	53





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Acq On : 5 Sep 2015 21:28
Operator : UM/IZ
Sample : G3555-01
Misc :
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Instrument : BNA_F
ClientSampleId : SB-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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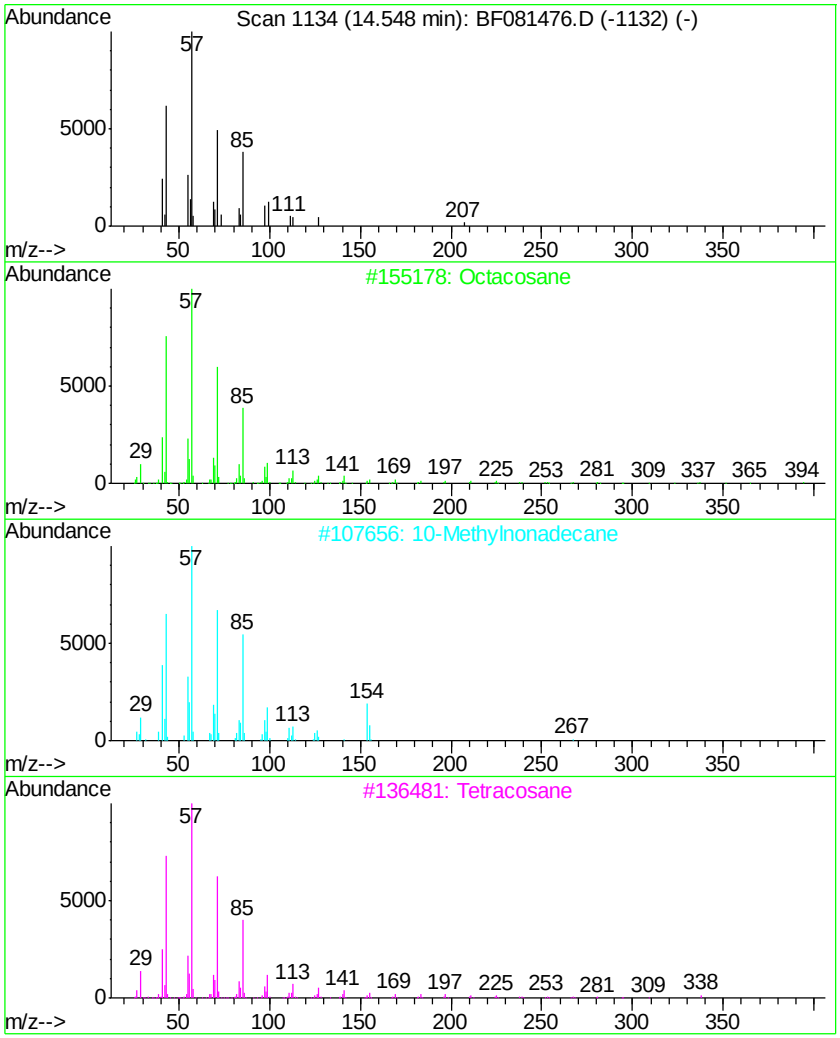
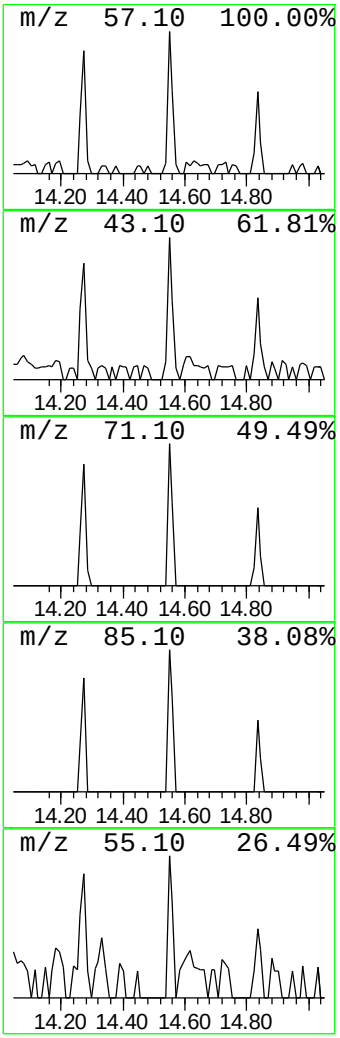
Peak Number 8 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.55	2.45 ng	28613	Perylene-d12	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	10-Methylnonadecane	282	C20H42	056862-62-5	86
3	Tetracosane	338	C24H50	000646-31-1	80
4	Tetratetracontane	619	C44H90	007098-22-8	80
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	78





Tentatively Identified Compound (LSC) summary

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Sample : G3555-01
Misc :
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Instrument : BNA_F
ClientSampleId : SB-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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...	4.40	54.2	ng	948077	1	6.35	349746	20.0
unknown6.12	6.12	95.1	ng	1662700	1	6.35	349746	20.0
Undecanoic acid	11.43	2.9	ng	63317	4	10.84	440696	20.0
Hexadecanoic acid...	12.29	5.5	ng	89844	5	13.45	328454	20.0
Octadecanoic acid...	12.99	4.1	ng	67579	5	13.45	328454	20.0
17-Pentatriacontene	13.36	8.0	ng	132070	5	13.45	328454	20.0
Octacosane	14.55	2.5	ng	28613	6	14.77	233256	20.0