LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081664.D
Acq On : 17 Sep 2015 3:37
Operator : UM/IZ
Sample : G3624-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-SOURCE-7

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	1.440	8	9	15	rBV	133083	363635	17.72%	1.771%
2	1.531	15	17	49	rVB	545947	1863758	90.82%	9.079%
3	3.280	168	170	182	rBB	40743	99333	4.84%	0.484%
4	4.491	270	276	298	rBV	356836	1164357	56.74%	5.672%
5	5.349	348	351	372	rBV	922262	1866827	90.97%	9.094%
6	7.612	544	549	552	rBV	942627	1869195	91.08%	9.105%
7	7.703	553	557	560	rVB	1089633	1900312	92.60%	9.257%
8	8.183	596	599	605	rVB	199032	317202	15.46%	1.545%
9	8.515	623	628	631	rBV	806259	1361436	66.34%	6.632%
10	9.486	708	713	716	rBV	635186	1223377	59.61%	5.959%
11	11.075	849	852	858	rBV	220198	405433	19.76%	1.975%
12	13.727	1079	1084	1087	rBV	1049868	2052154	100.00%	9.997%
13	14.778	1172	1176	1186	rBB	210203	342808	16.70%	1.670%
14	15.212	1210	1214	1219	rBB	257503	433565	21.13%	2.112%
15	16.618	1333	1337	1340	rBB	16101	27939	1.36%	0.136%
16	17.121	1376	1381	1384	rBV	726304	1316969	64.17%	6.415%
17	17.750	1432	1436	1444	rBV	21506	54713	2.67%	0.267%
18	18.710	1516	1520	1524	rBV	256535	452544	22.05%	2.204%
19	18.836	1528	1531	1534	rBV2	18768	33767	1.65%	0.164%
20	19.876	1618	1622	1625	rBB	10598	20702	1.01%	0.101%
21	20.482	1671	1675	1688	rBV	77141	177530	8.65%	0.865%
22	21.876	1794	1797	1803	rBV	17690	31439	1.53%	0.153%
23	22.082	1811	1815	1818	rBV	1385295	2004522	97.68%	9.765%
24	22.550	1850	1856	1858	rBV2	7645	20536	1.00%	0.100%
25	23.350	1917	1926	1929	rBV	416405	626281	30.52%	3.051%
26	24.013	1982	1984	1991	rBV2	21162	47952	2.34%	0.234%
27	24.368	2013	2015	2018	rBV	18287	26680	1.30%	0.130%
28	24.608	2034	2036	2038	rBV	27670	35824	1.75%	0.175%
29	24.791	2049	2052	2056	rVB	257255	268199	13.07%	1.306%
30	25.191	2084	2087	2089	rBV	19003	23180	1.13%	0.113%
31	25.236	2089	2091	2100	rVB3	24548	65704	3.20%	0.320%
32	26.219	2174	2177	2182	rBV4	10434	30785	1.50%	0.150%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081664.D
Acq On : 17 Sep 2015 3:37
Operator : UM/IZ
Sample : G3624-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-SOURCE-7

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

Sum of corrected areas: 20528658

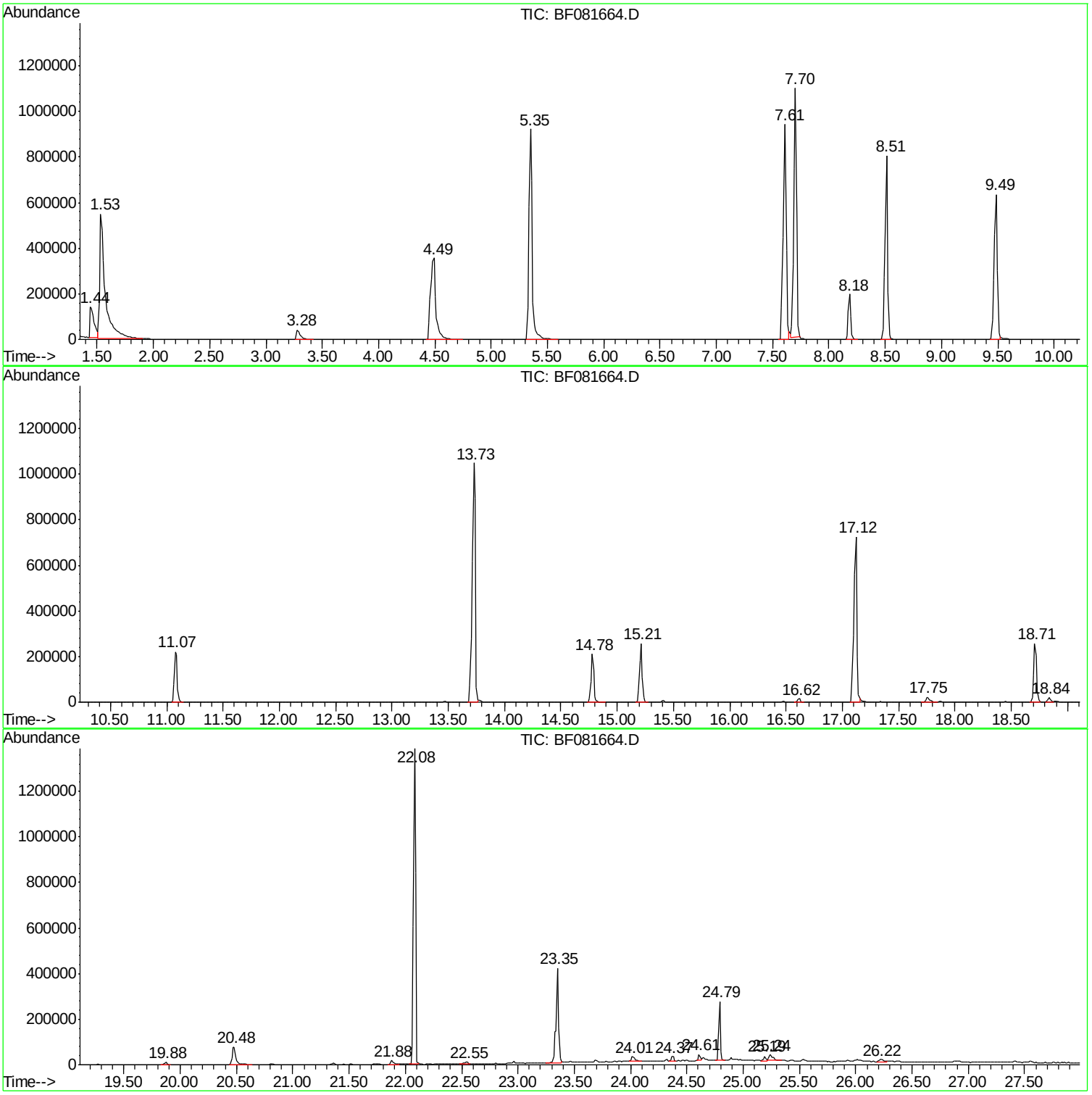
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081664.D
Acq On : 17 Sep 2015 3:37
Operator : UM/IZ
Sample : G3624-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-SOURCE-7

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081664.D
Acq On : 17 Sep 2015 3:37
Operator : UM/IZ
Sample : G3624-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-SOURCE-7

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

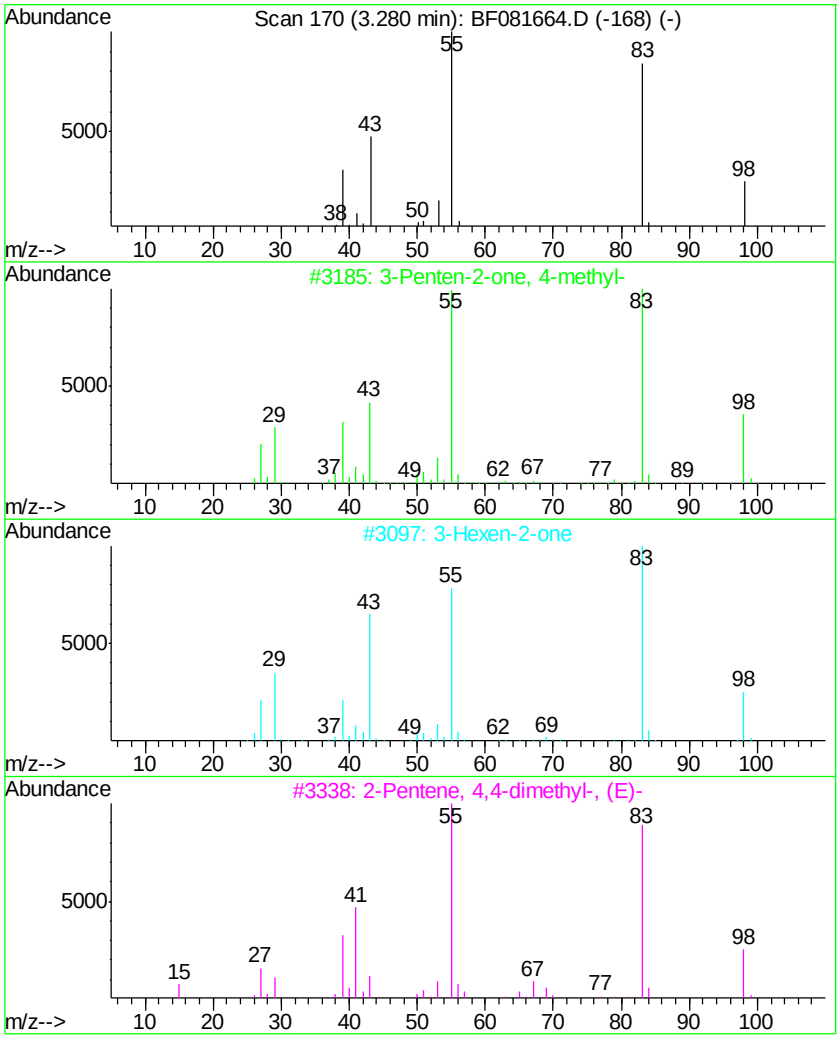
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

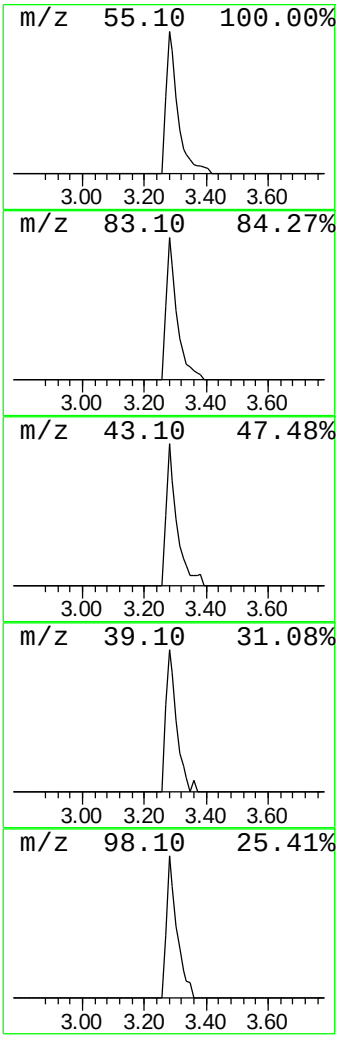
****

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.28	6.26 ng	99333	1,4-Dichlorobenzene-d4	8.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2	3-Hexen-2-one	98	C6H10O	000763-93-9	86
3	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	80
4	3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	72
5	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	64





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081664.D
Acq On : 17 Sep 2015 3:37
Operator : UM/IZ
Sample : G3624-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-SOURCE-7

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

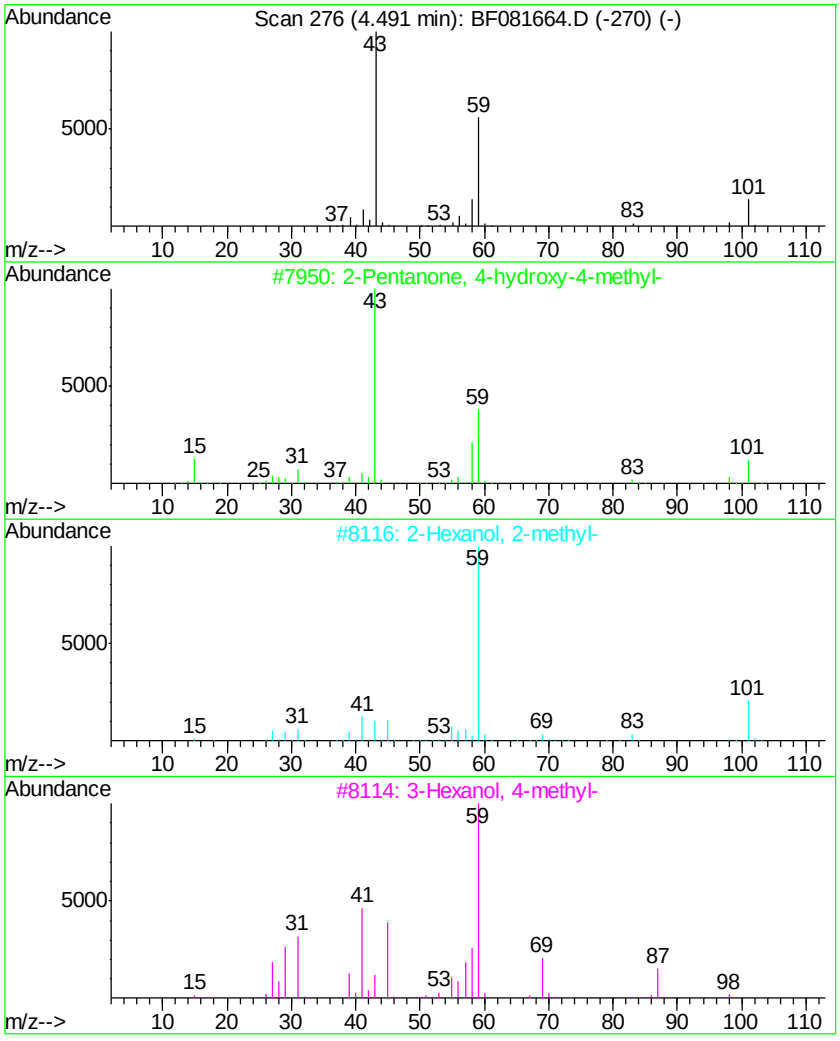
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

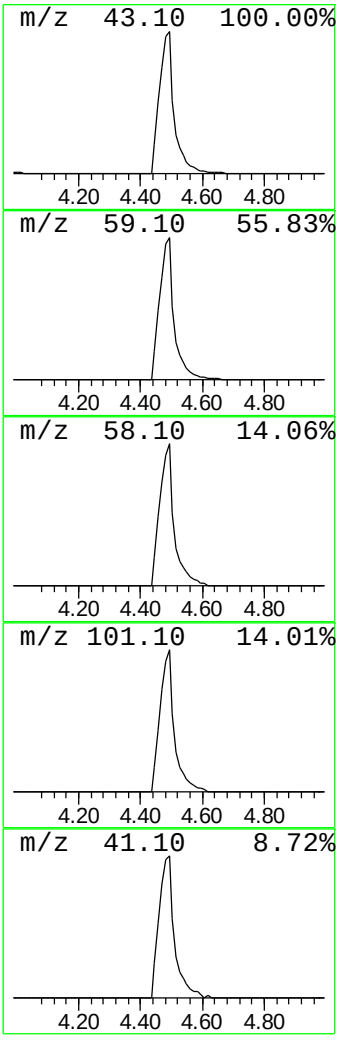
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.49	73.41 ng	1164360	1,4-Dichlorobenzene-d4	8.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
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Acq On : 17 Sep 2015 3:37
Operator : UM/IZ
Sample : G3624-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-SOURCE-7

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

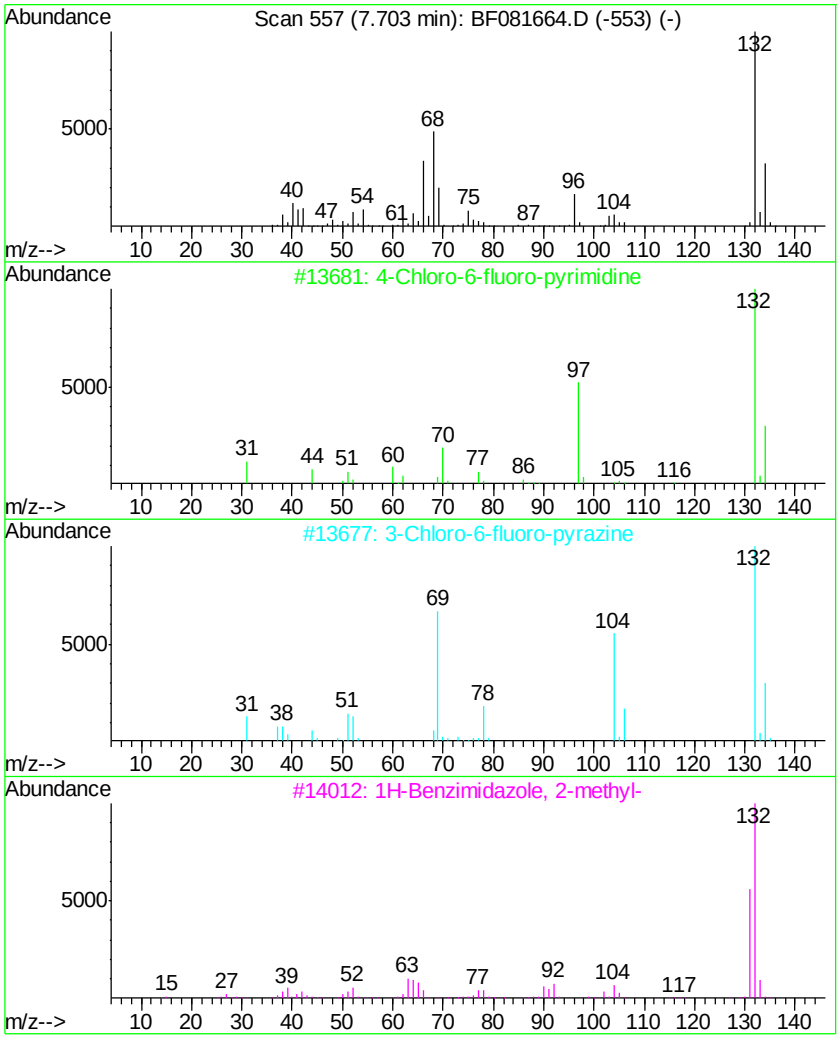
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

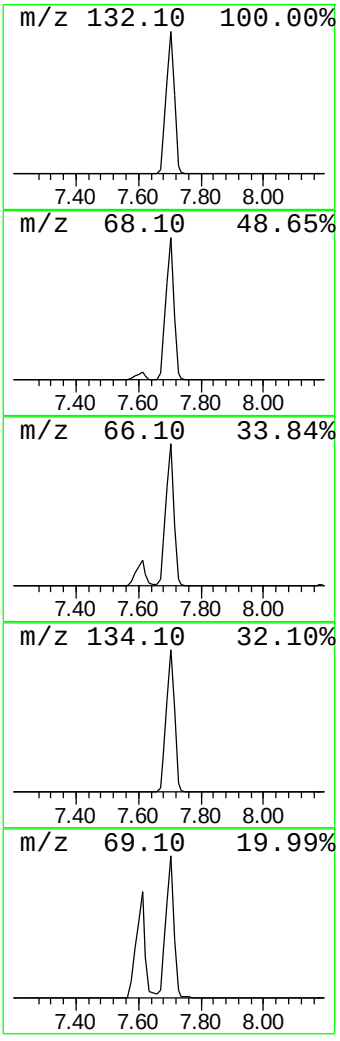
****

Peak Number 5 unknown7.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	119.82 ng	1900310	1,4-Dichlorobenzene-d4	8.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081664.D
Acq On : 17 Sep 2015 3:37
Operator : UM/IZ
Sample : G3624-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-SOURCE-7

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

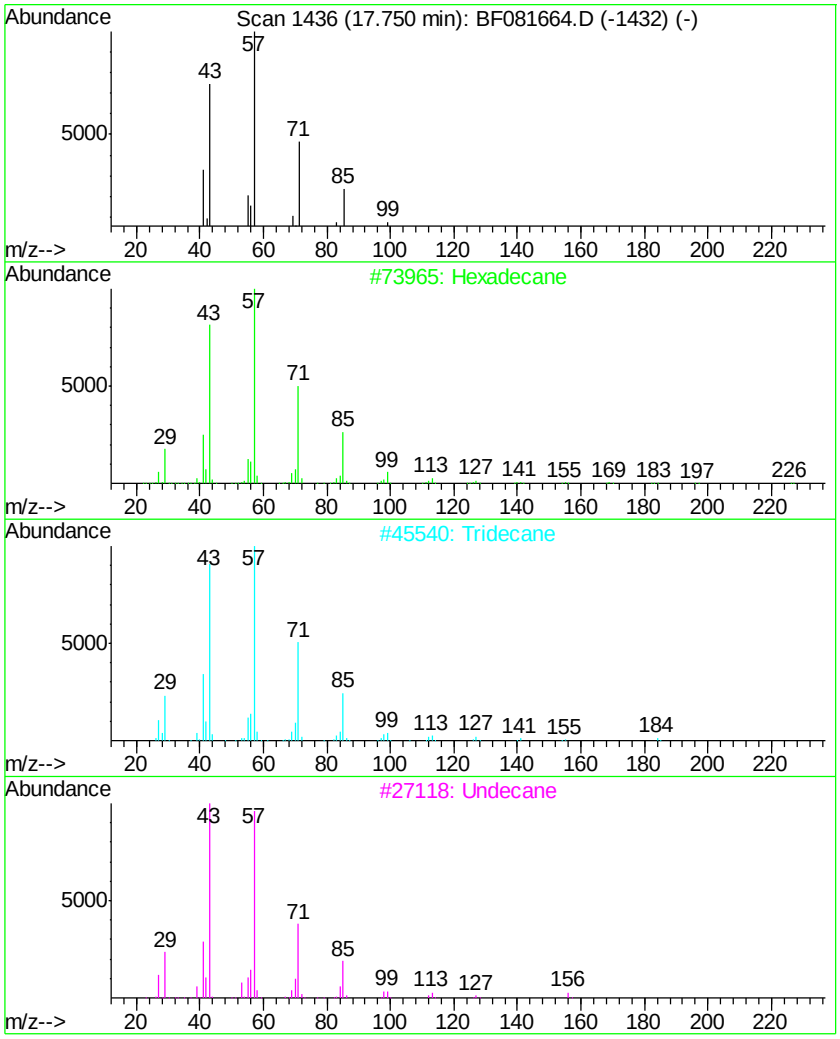
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

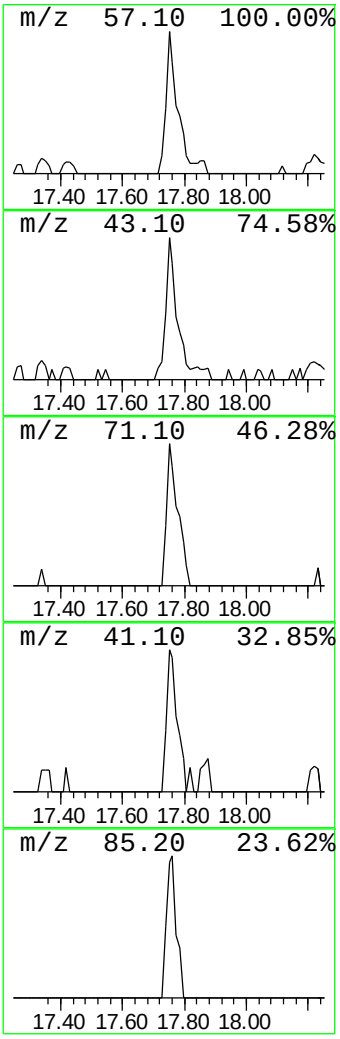
****

Peak Number 7 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.75	2.42 ng	54713	Phenanthrene-d10	18.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	83
2	Tridecane	184	C13H28	000629-50-5	78
3	Undecane	156	C11H24	001120-21-4	64
4	Ether, hexyl pentyl	172	C11H24O	032357-83-8	56
5	Heptane, 4-ethyl-	128	C9H20	002216-32-2	42





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081664.D
Acq On : 17 Sep 2015 3:37
Operator : UM/IZ
Sample : G3624-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-SOURCE-7

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

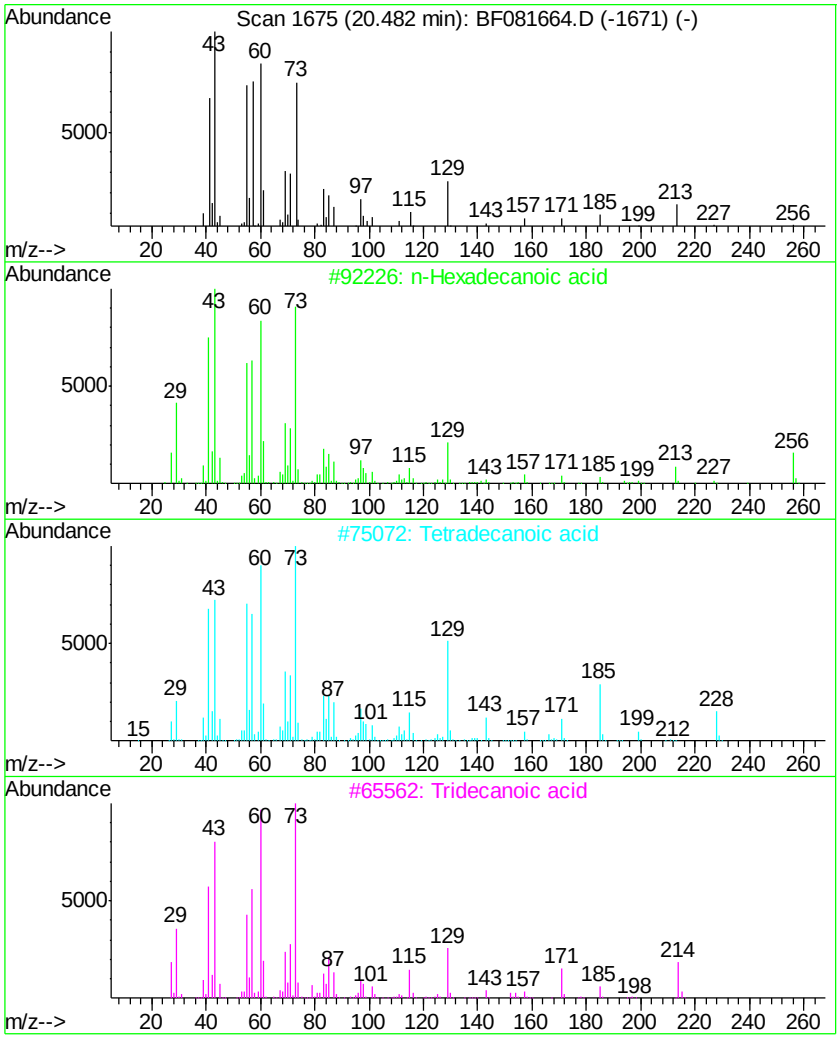
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

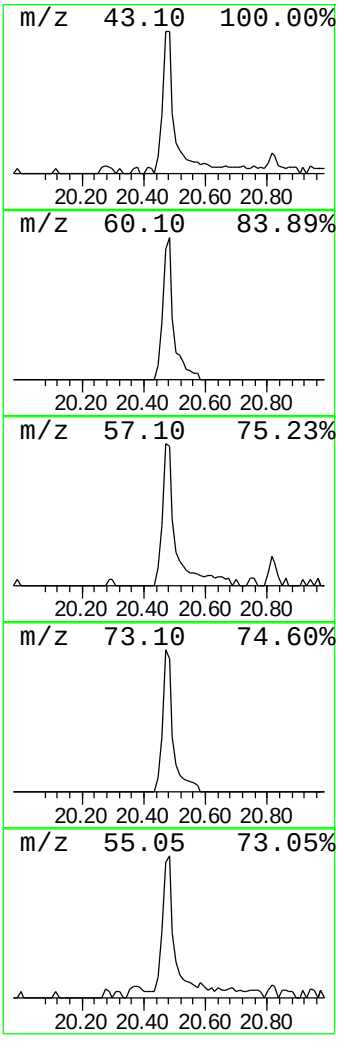
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.48	7.85 ng	177530	Phenanthrene-d10	18.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	Undecanoic acid	186	C11H22O2	000112-37-8	58
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081664.D
Acq On : 17 Sep 2015 3:37
Operator : UM/IZ
Sample : G3624-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-SOURCE-7

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

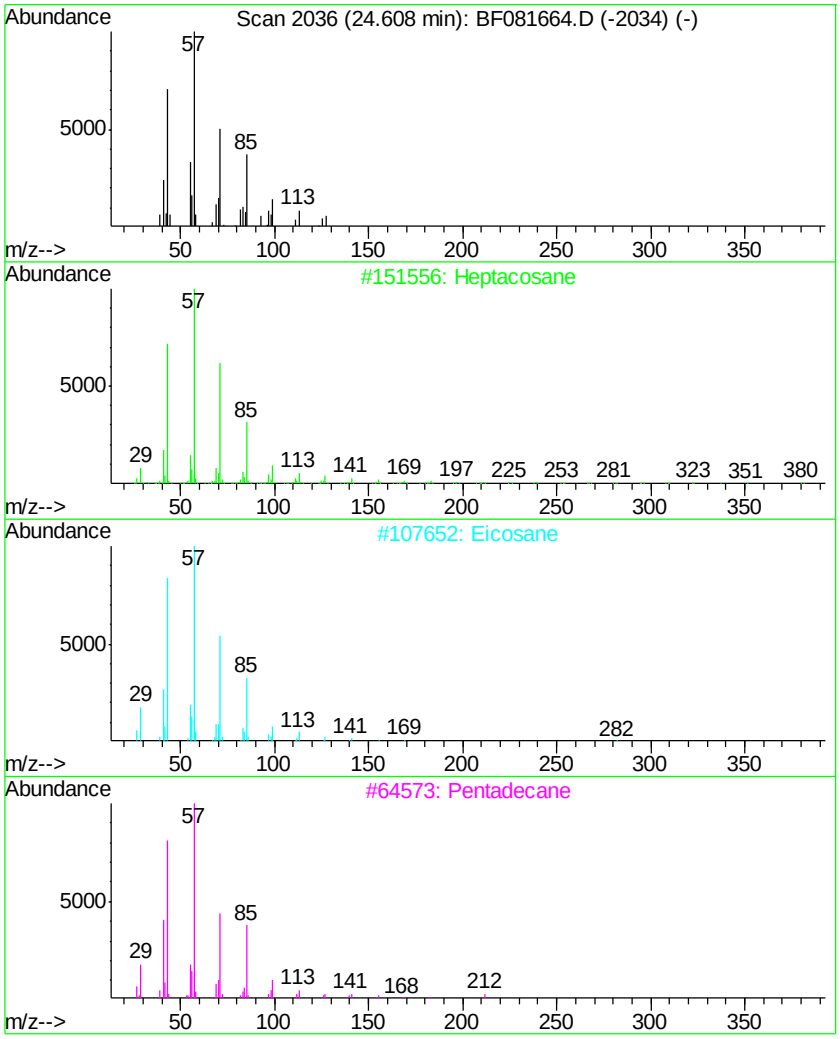
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

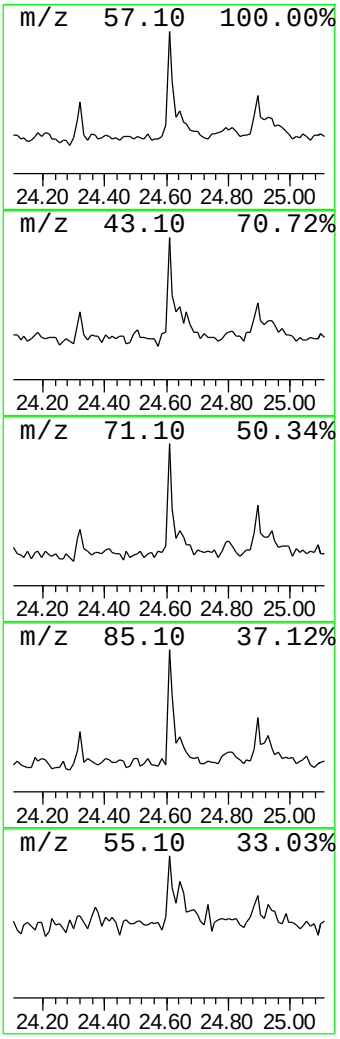
****

Peak Number 9 Heptacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.61	2.67 ng	35824	Perylene-d12	24.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	83
2	Eicosane	282	C20H42	000112-95-8	80
3	Pentadecane	212	C15H32	000629-62-9	80
4	Hexadecane	226	C16H34	000544-76-3	78
5	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	78





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081664.D
Acq On : 17 Sep 2015 3:37
Operator : UM/IZ
Sample : G3624-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-SOURCE-7

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

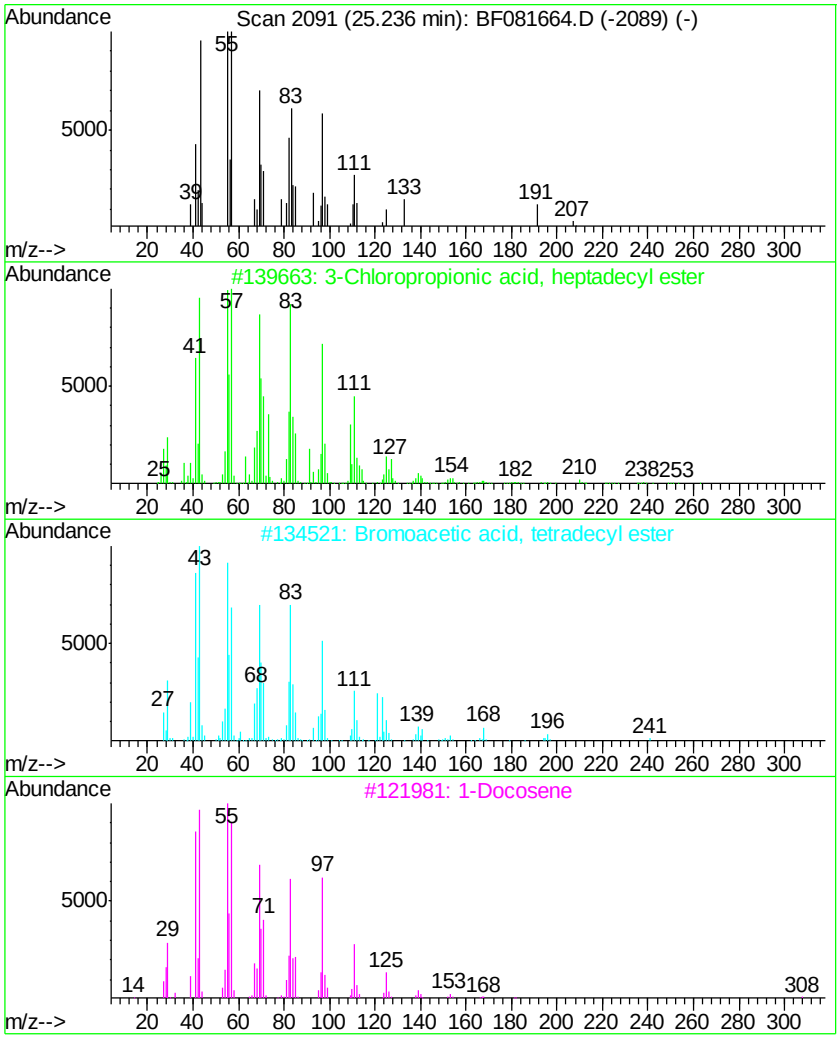
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

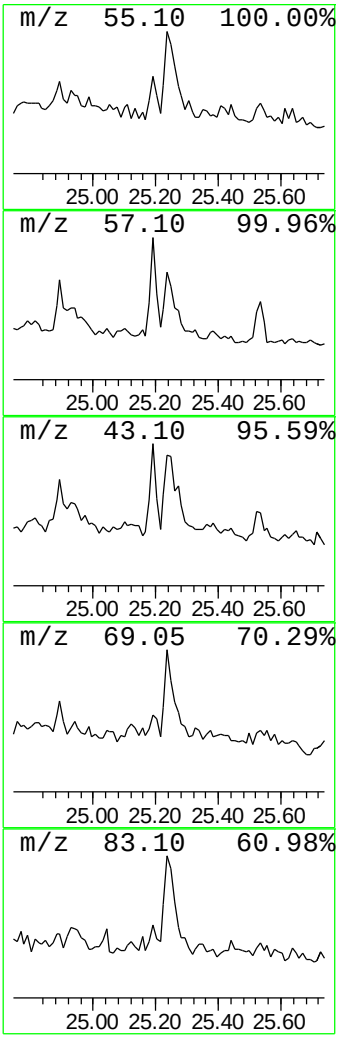
****

Peak Number 10 3-Chloropropionic acid, hep... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.24	4.90 ng	65704	Perylene-d12	24.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	81
2	Bromoacetic acid, tetradecyl ester	334	C16H31BrO2	018992-01-3	76
3	1-Docosene	308	C22H44	001599-67-3	76
4	1-Heptadecanol	256	C17H36O	001454-85-9	76
5	1-Hexadecanol	242	C16H34O	036653-82-4	76





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
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Acq On : 17 Sep 2015 3:37
Operator : UM/IZ
Sample : G3624-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-SOURCE-7

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

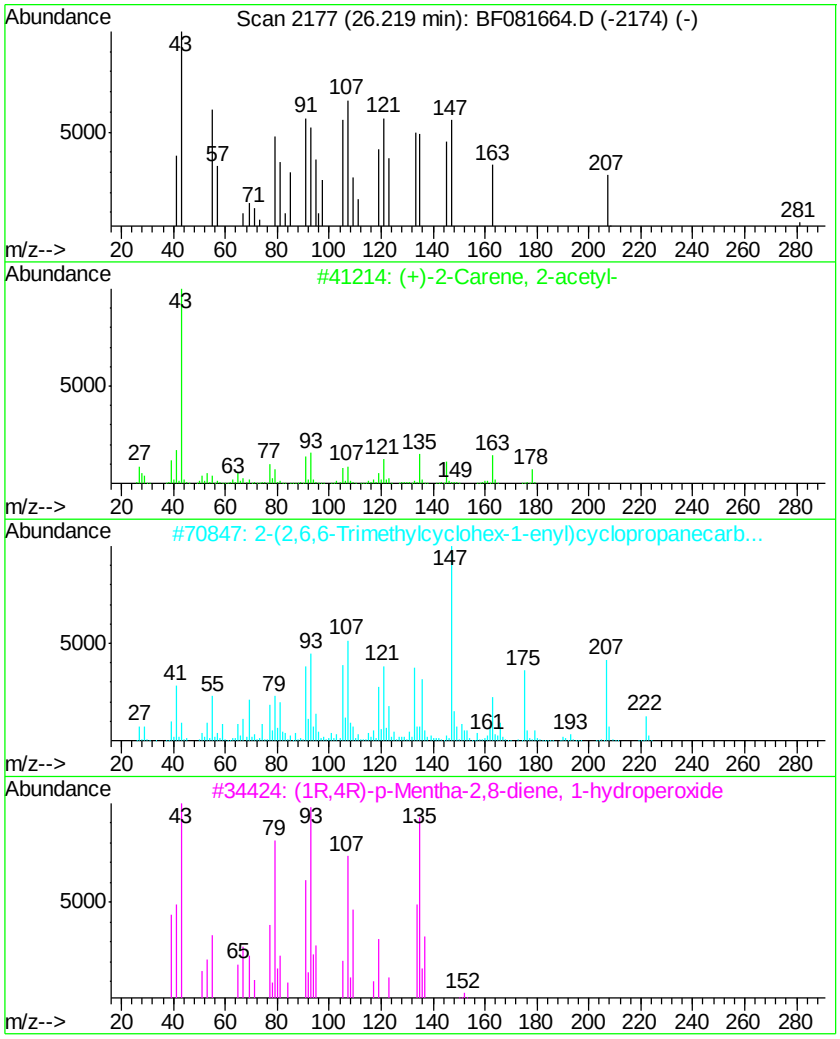
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

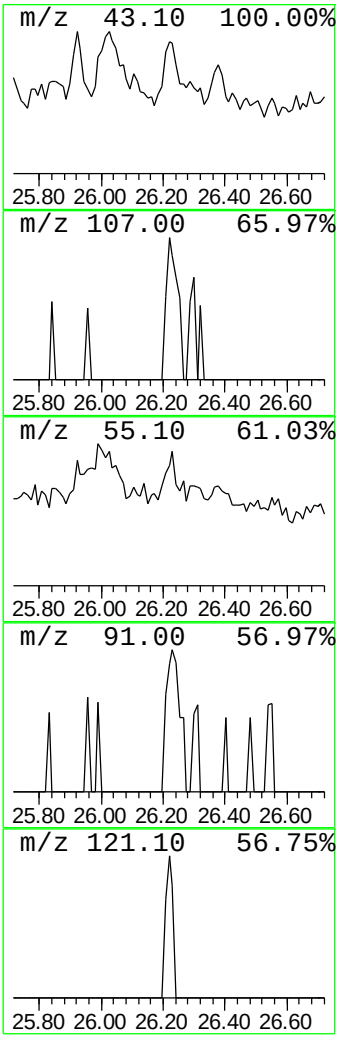
****

Peak Number 11 unknown26.22 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.22	2.30 ng	30785	Perylene-d12	24.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-2-Carene, 2-acetyl-	178	C12H18O	1000151-09-7	27
2	2-(2,6,6-Trimethylcyclohex-1-eny...	222	C14H22O2	1000185-64-1	23
3	(1R,4R)-p-Mentha-2,8-diene, 1-hy...	168	C10H16O2	1000292-74-0	12
4	.alpha.-Farnesene	204	C15H24	000502-61-4	10
5	Bronopol	199	C3H6BrNO4	000052-51-7	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081664.D
Acq On : 17 Sep 2015 3:37
Operator : UM/IZ
Sample : G3624-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-SOURCE-7

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
3-Penten-2-one, 4...	3.28	6.3	ng	99333	1	8.18	317202	20.0
2-Pentanone, 4-hy...	4.49	73.4	ng	1164360	1	8.18	317202	20.0
unknown7.70	7.70	119.8	ng	1900310	1	8.18	317202	20.0
Hexadecane	17.75	2.4	ng	54713	4	18.71	452544	20.0
n-Hexadecanoic acid	20.48	7.8	ng	177530	4	18.71	452544	20.0
Heptacosane	24.61	2.7	ng	35824	6	24.79	268199	20.0
3-Chloropropionic...	25.24	4.9	ng	65704	6	24.79	268199	20.0
unknown26.22	26.22	2.3	ng	30785	6	24.79	268199	20.0