LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF021318\
Data File : BF102961.D
Acq On : 13 Feb 2018 15:03
Operator : SJ/JU
Sample : J1397-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-021218-B

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-BF020318.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	2.140	4	9	23	rVB	774304	991299	23.40%	2.671%
2	3.951	313	317	322	rVB	48939	62637	1.48%	0.169%
3	5.104	510	513	524	rVB	106588	141332	3.34%	0.381%
4	5.493	574	579	582	rBV	3948338	3974302	93.81%	10.708%
5	6.504	745	751	755	rBV	3697983	4236501	100.00%	11.414%
6	6.645	770	775	778	rBV	3960510	3992715	94.25%	10.757%
7	6.869	810	813	817	rBV	1180677	1017152	24.01%	2.740%
8	7.028	836	840	843	rBV	3236007	2878610	67.95%	7.756%
9	7.434	904	909	912	rBV	2644357	2692361	63.55%	7.254%
10	7.504	918	921	935	rVB	38107	51632	1.22%	0.139%
11	8.151	1028	1031	1035	rBV	1522440	1390417	32.82%	3.746%
12	9.228	1209	1214	1217	rBV	4015601	3763346	88.83%	10.139%
13	9.298	1223	1226	1229	rVB	66778	55994	1.32%	0.151%
14	9.616	1277	1280	1283	rBV	343746	307053	7.25%	0.827%
15	9.828	1309	1316	1321	rBV	211510	215855	5.10%	0.582%
16	9.910	1326	1330	1334	rVV	1694964	1506189	35.55%	4.058%
17	10.151	1368	1371	1375	rBV3	50376	49548	1.17%	0.133%
18	10.328	1399	1401	1404	rVB	237072	193422	4.57%	0.521%
19	10.551	1432	1439	1441	rBV	68243	91254	2.15%	0.246%
20	10.698	1460	1464	1467	rBV	2472723	2307426	54.47%	6.217%
21	10.804	1479	1482	1492	rVB	206951	234817	5.54%	0.633%
22	11.251	1555	1558	1560	rBV	114116	92974	2.19%	0.250%
23	11.280	1560	1563	1569	rVB3	44768	60673	1.43%	0.163%
24	11.398	1579	1583	1585	rBV	1403707	1346548	31.78%	3.628%
25	11.416	1585	1586	1589	rVB	103403	73347	1.73%	0.198%
26	11.674	1628	1630	1633	rVB	59817	46510	1.10%	0.125%
27	11.910	1665	1670	1679	rBV3	105992	142914	3.37%	0.385%
28	12.080	1697	1699	1705	rVB	49273	43095	1.02%	0.116%
29	12.463	1762	1764	1766	rBV2	89506	93720	2.21%	0.253%
30	12.480	1766	1767	1772	rVB3	83822	73298	1.73%	0.197%
31	12.604	1785	1788	1793	rVB	125048	111126	2.62%	0.299%
32	12.833	1822	1827	1830	rBV	115013	137068	3.24%	0.369%
33	12.974	1847	1851	1855	rBV	2538661	2513249	59.32%	6.771%
34	13.857	1998	2001	2009	rVB	264877	292140	6.90%	0.787%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF021318\
Data File : BF102961.D
Acq On : 13 Feb 2018 15:03
Operator : SJ/JU
Sample : J1397-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-021218-B

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-BF020318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.033	2026	2031	2034	rBV	854608	903900	21.34%	2.435%
36	15.068	2205	2207	2211	rBV	40749	56363	1.33%	0.152%
37	15.133	2215	2218	2223	rBV4	36246	48377	1.14%	0.130%
38	15.504	2276	2281	2291	rVB	719975	926983	21.88%	2.498%

Sum of corrected areas: 37116147

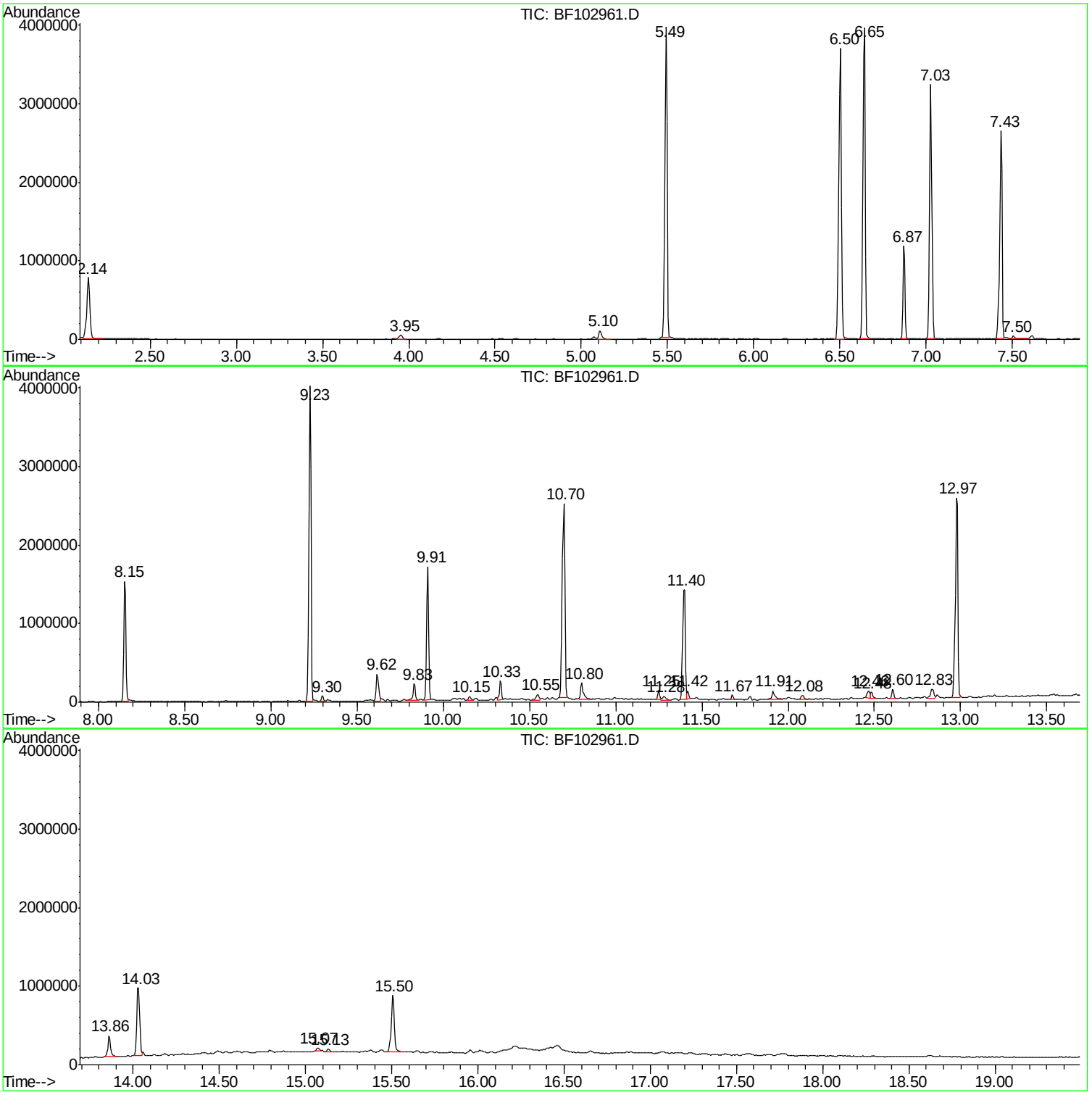
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF021318\
Data File : BF102961.D
Acq On : 13 Feb 2018 15:03
Operator : SJ/JU
Sample : J1397-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-021218-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF021318\
Data File : BF102961.D
Acq On : 13 Feb 2018 15:03
Operator : SJ/JU
Sample : J1397-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-021218-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

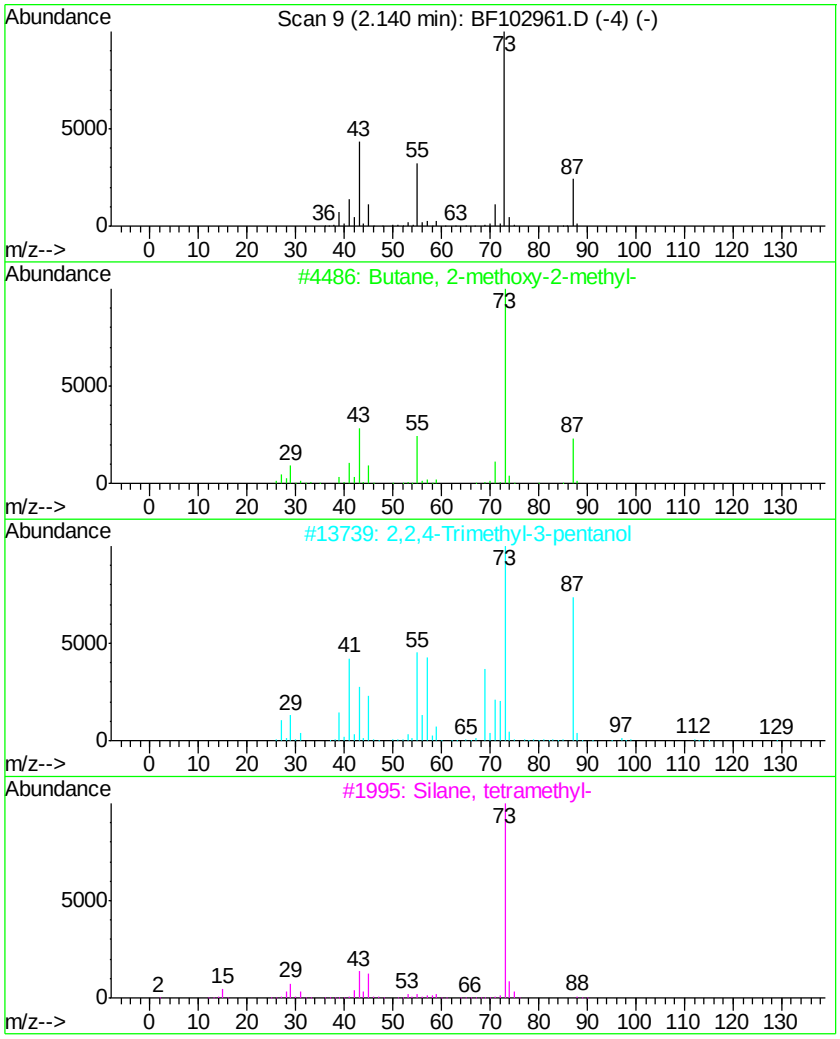
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

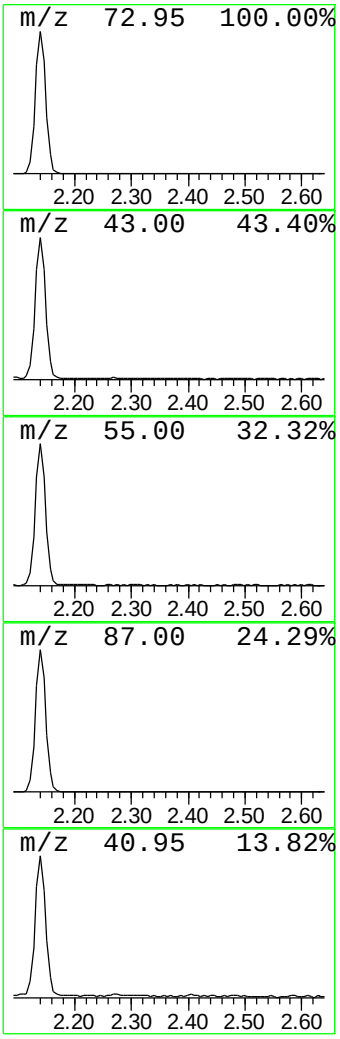
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	19.49 ng	991299	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\HPCHEM1\BNA F\DATA\BF021318\
Data File : BF102961.D
Acq On : 13 Feb 2018 15:03
Operator : SJ/JU
Sample : J1397-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-021218-B

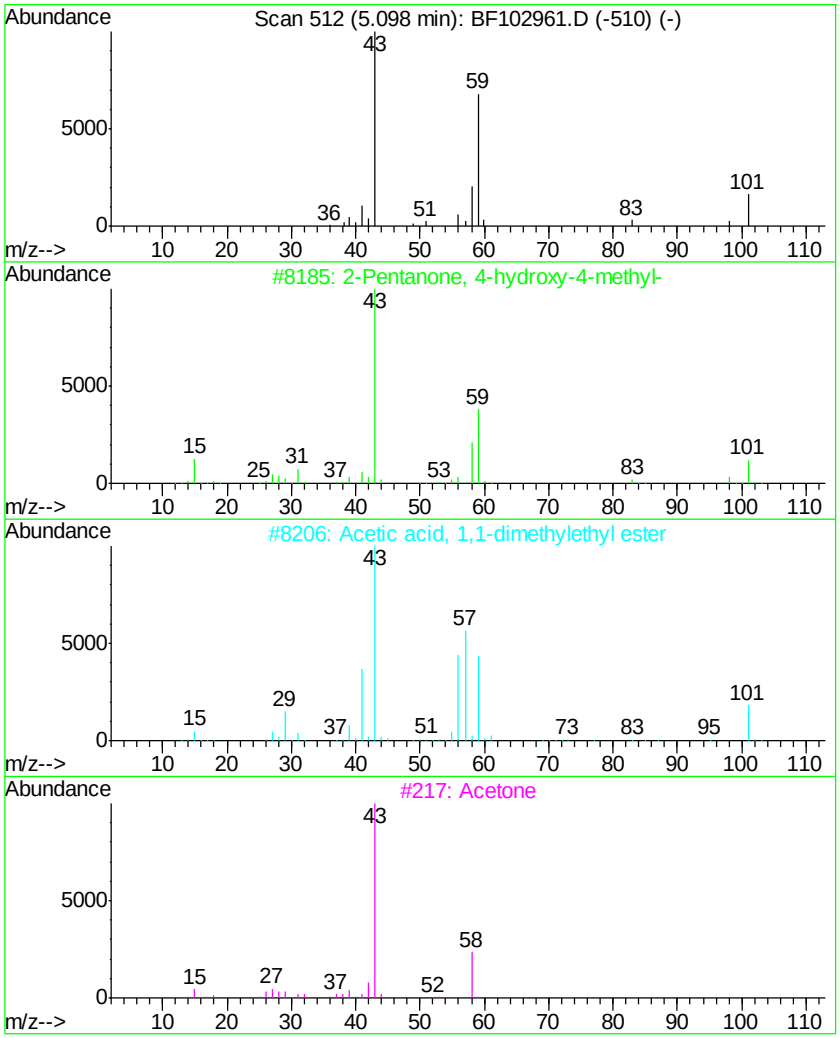
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

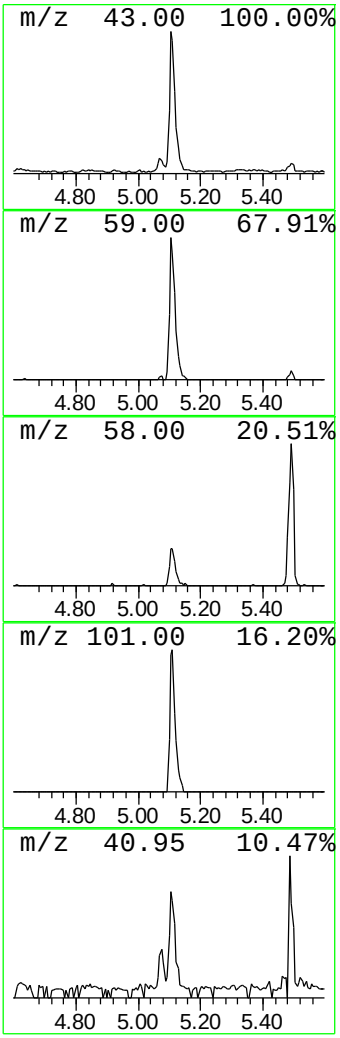
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	2.78 ng	141332	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Acetone	58	C3H6O	000067-64-1	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF021318\
Data File : BF102961.D
Acq On : 13 Feb 2018 15:03
Operator : SJ/JU
Sample : J1397-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-021218-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

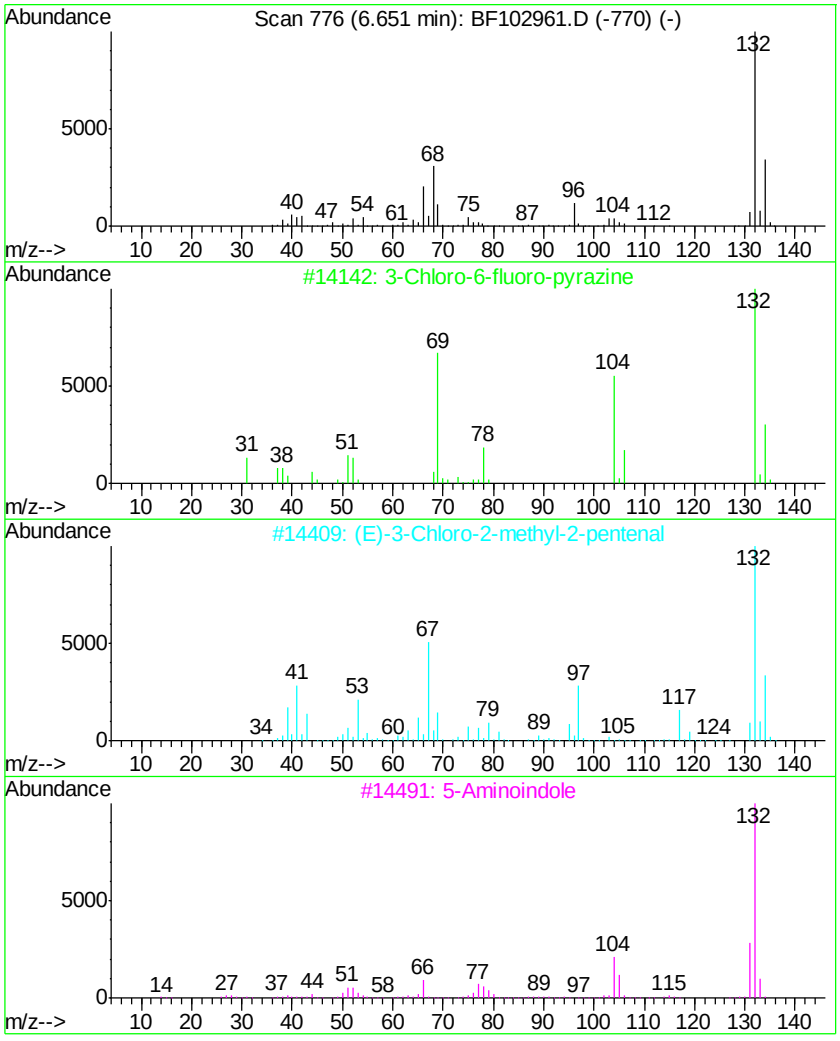
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

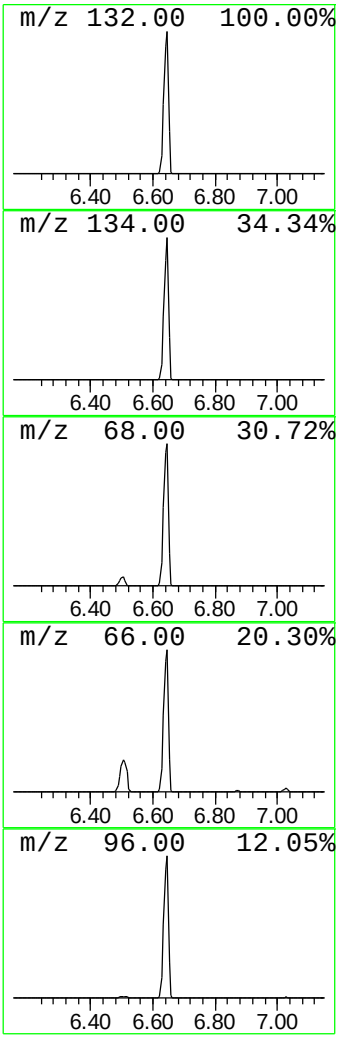
****

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	78.51 ng	3992720	1,4-Dichlorobenzene-d4	6.87

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	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF021318\
Data File : BF102961.D
Acq On : 13 Feb 2018 15:03
Operator : SJ/JU
Sample : J1397-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-021218-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

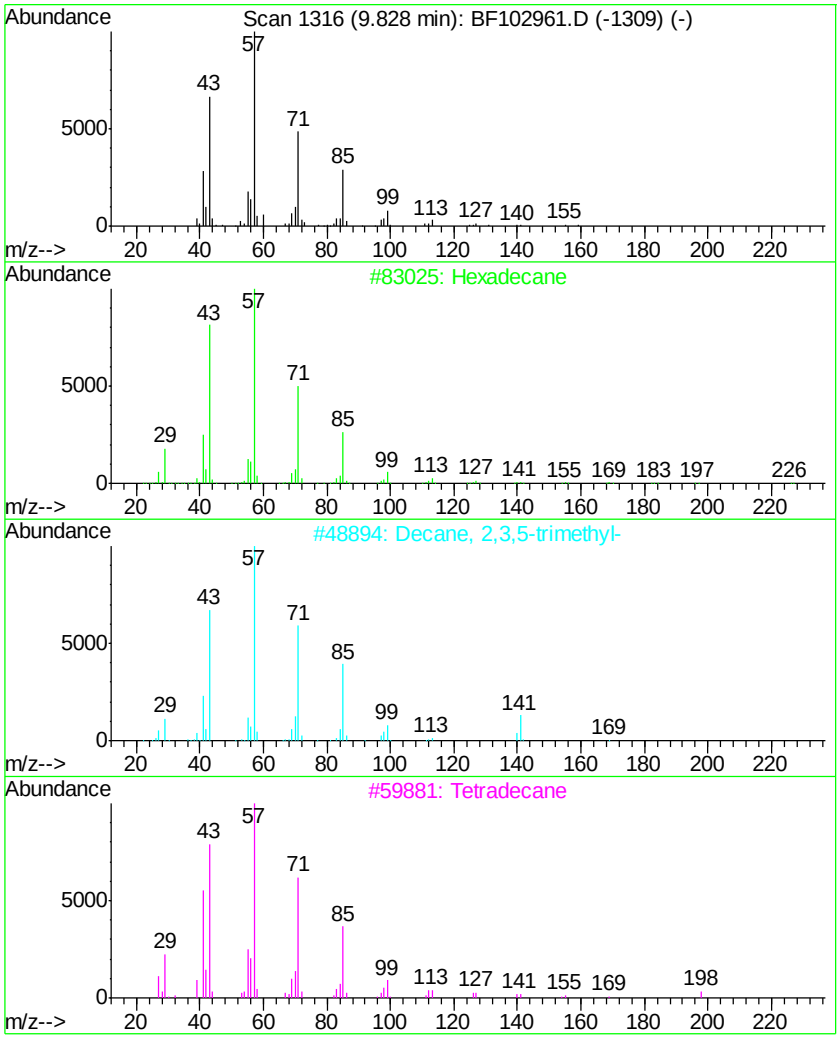
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

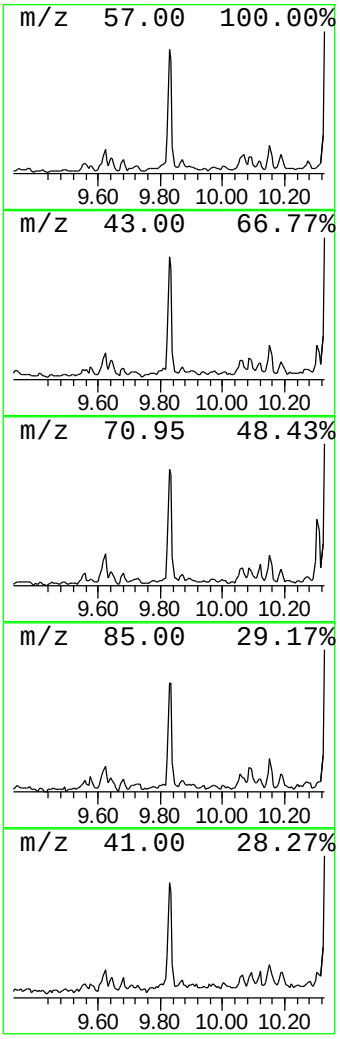
****

Peak Number 5 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.83	2.87 ng	215855	Acenaphthene-d10	9.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	80
3	Tetradecane	198	C14H30	000629-59-4	72
4	Heneicosane	296	C21H44	000629-94-7	72
5	Pentadecane	212	C15H32	000629-62-9	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF021318\
Data File : BF102961.D
Acq On : 13 Feb 2018 15:03
Operator : SJ/JU
Sample : J1397-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-021218-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

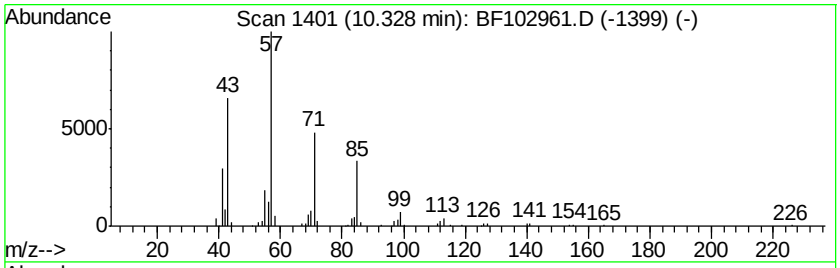
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

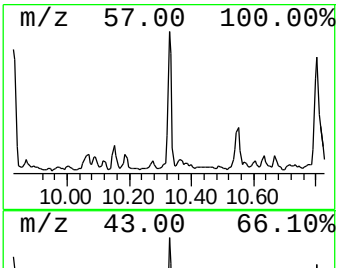
****

Peak Number 6 Tetradecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.33	2.57 ng	193422	Acenaphthene-d10	9.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	90
2	Tridecane	184	C13H28	000629-50-5	90
3	Hexadecane	226	C16H34	000544-76-3	90
4	Pentadecane	212	C15H32	000629-62-9	90
5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF021318\
Data File : BF102961.D
Acq On : 13 Feb 2018 15:03
Operator : SJ/JU
Sample : J1397-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-021218-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

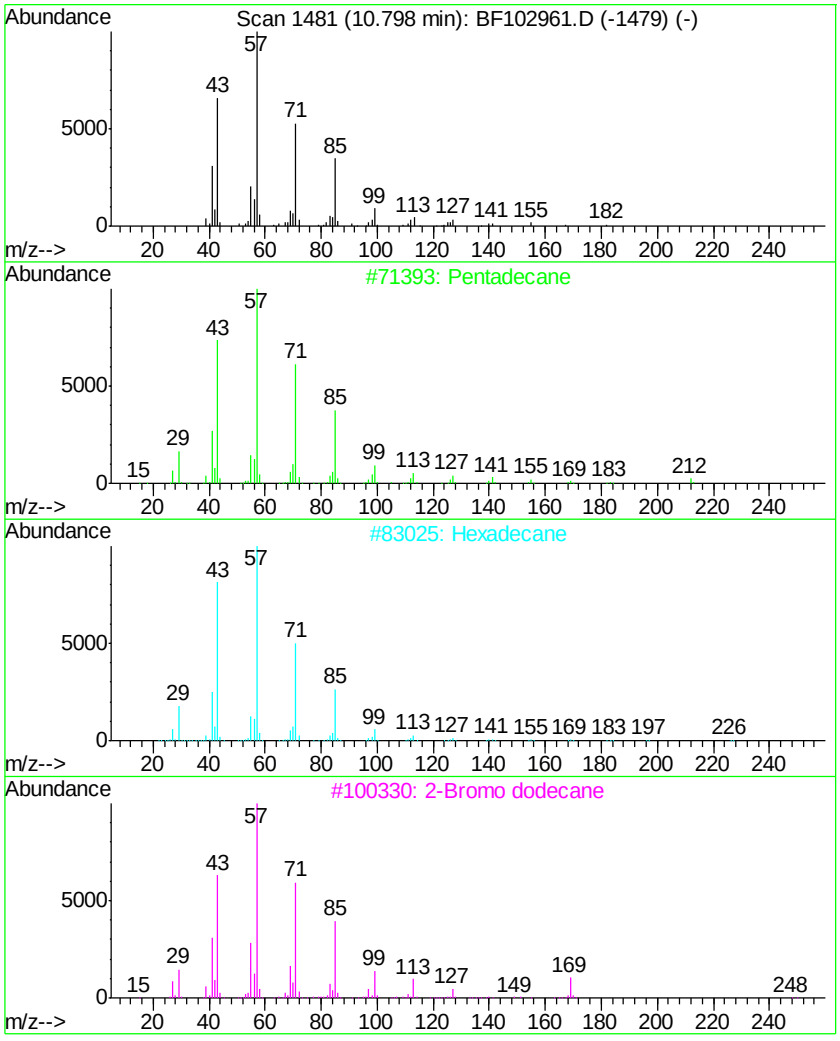
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

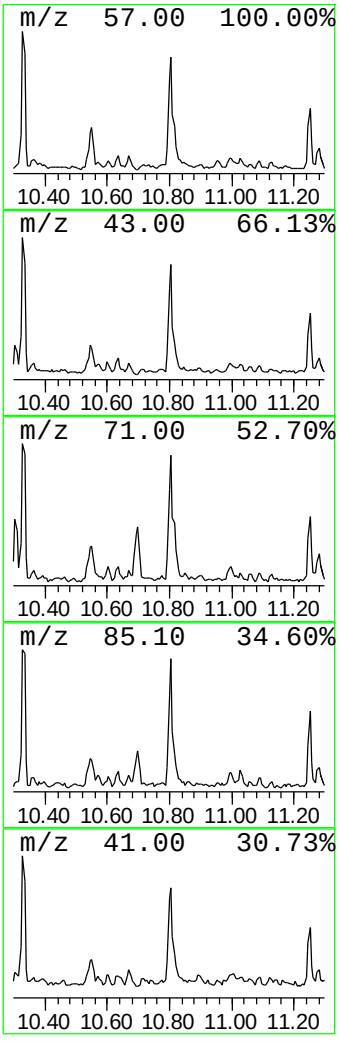
****

Peak Number 7 Pentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	3.49 ng	234817	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	90
4	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86
5	Bacchotricuneatin c	342	C20H22O5	066563-30-2	68





Data Path : Z:\HPCHEM1\BNA F\DATA\BF021318\
Data File : BF102961.D
Acq On : 13 Feb 2018 15:03
Operator : SJ/JU
Sample : J1397-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-021218-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

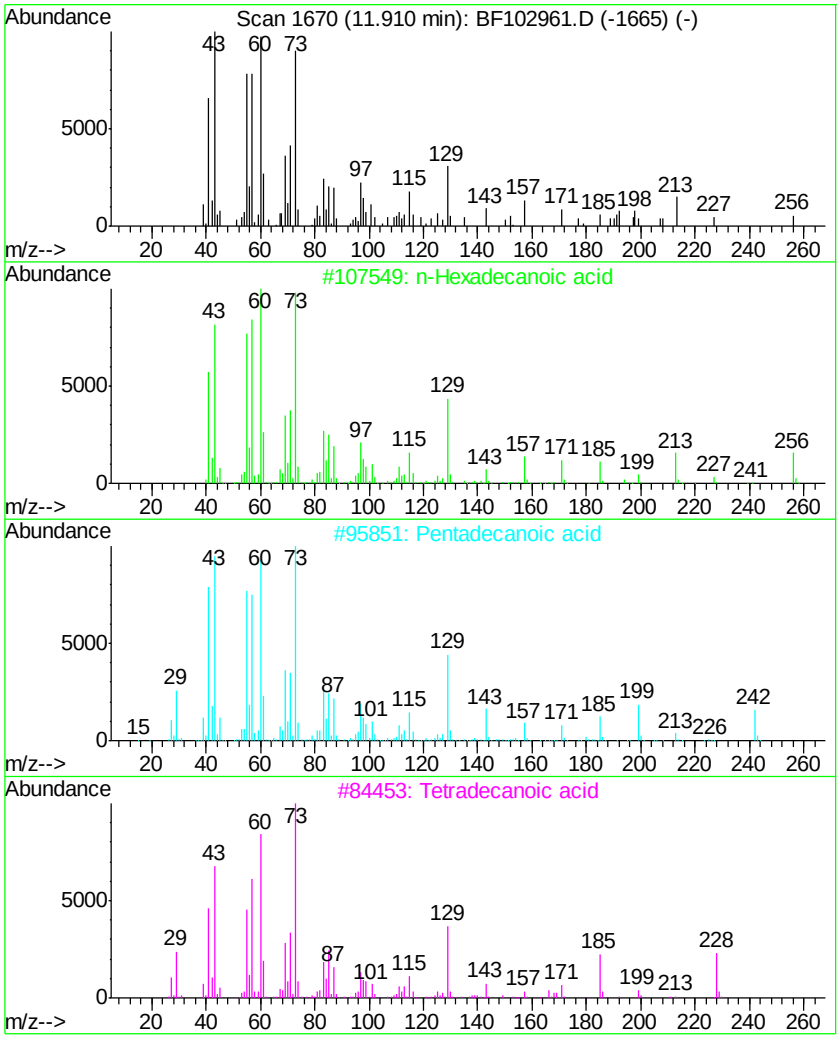
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

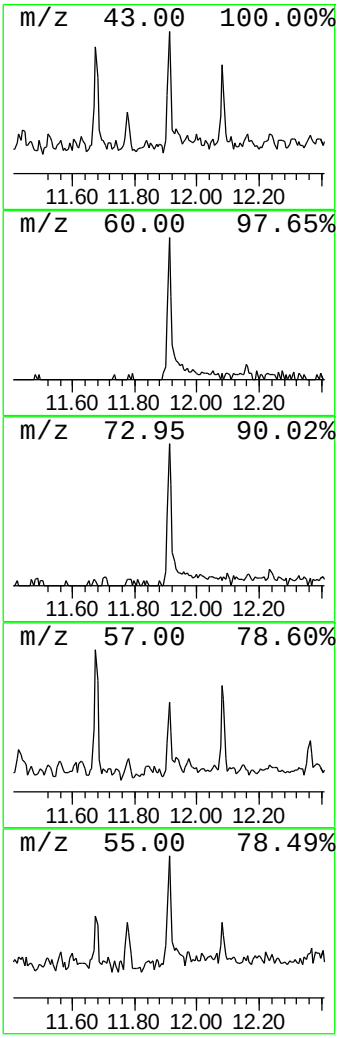
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	2.12 ng	142914	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	N-Cyclooct-4-enylacetamide	167	C10H17NO	170952-69-9	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF021318\
Data File : BF102961.D
Acq On : 13 Feb 2018 15:03
Operator : SJ/JU
Sample : J1397-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-021218-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

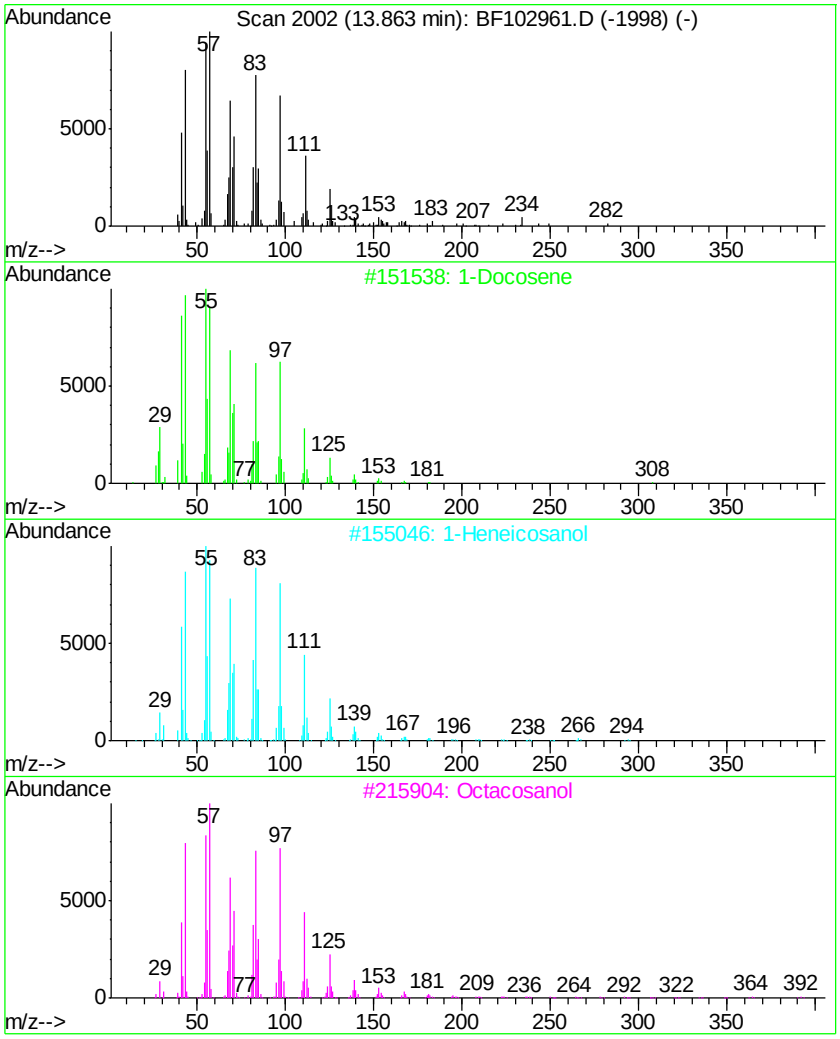
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

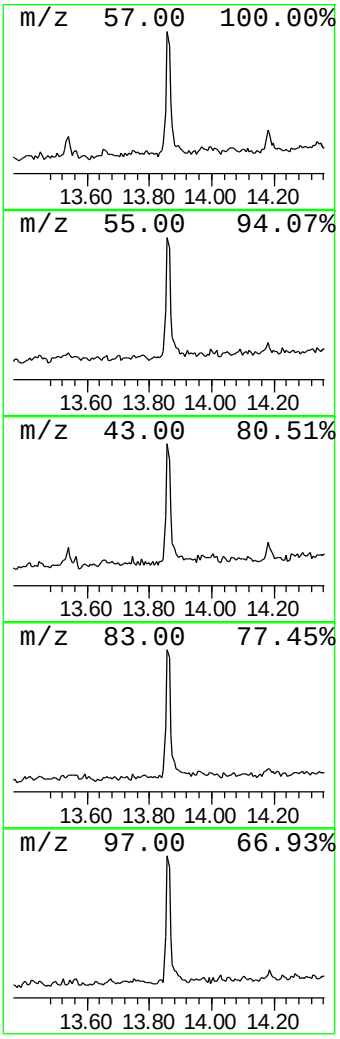
****

Peak Number 10 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	6.46 ng	292140	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	91
3	Octacosanol	410	C28H58O	000557-61-9	91
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021318\
Data File : BF102961.D
Acq On : 13 Feb 2018 15:03
Operator : SJ/JU
Sample : J1397-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-021218-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.14	19.5	ng	991299	1	6.87	1017150	20.0
2-Pentanone, 4-hy...	5.10	2.8	ng	141332	1	6.87	1017150	20.0
unknown6.65	6.65	78.5	ng	3992720	1	6.87	1017150	20.0
Hexadecane	9.83	2.9	ng	215855	3	9.91	1506190	20.0
Tetradecane	10.33	2.6	ng	193422	3	9.91	1506190	20.0
Pentadecane	10.80	3.5	ng	234817	4	11.40	1346550	20.0
n-Hexadecanoic acid	11.91	2.1	ng	142914	4	11.40	1346550	20.0
1-Docosene	13.86	6.5	ng	292140	5	14.03	903900	20.0