LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102717\
Data File : BF099879.D
Acq On : 27 Oct 2017 16:06
Operator : SJ/JU
Sample : I6112-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-MARION26KV-(2-3)

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-BF102317.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	5.016	495	498	516	rBV	228409	409394	13.63%	1.635%
2	5.422	563	567	594	rVB	2101605	2259213	75.22%	9.022%
3	6.445	736	741	758	rBV	2018634	2421724	80.63%	9.671%
4	6.569	758	762	765	rBV	2459618	2365069	78.74%	9.445%
5	6.793	797	800	808	rBV	604740	515586	17.17%	2.059%
6	6.951	823	827	830	rBV	2136309	1913345	63.70%	7.641%
7	7.369	893	898	908	rBV	1455128	1501759	50.00%	5.997%
8	8.075	1015	1018	1030	rVB	839358	740348	24.65%	2.957%
9	8.639	1110	1114	1123	rBV	225321	222011	7.39%	0.887%
10	9.157	1196	1202	1205	rBV	3090686	3003645	100.00%	11.995%
11	9.557	1265	1270	1273	rBV	955130	816517	27.18%	3.261%
12	9.839	1312	1318	1322	rBV	903946	817659	27.22%	3.265%
13	10.557	1435	1440	1443	rBV	1109243	930472	30.98%	3.716%
14	10.639	1449	1454	1457	rBV	1566122	1530306	50.95%	6.111%
15	10.739	1466	1471	1475	rBV5	24311	35440	1.18%	0.142%
16	10.886	1492	1496	1500	rBV	68052	56197	1.87%	0.224%
17	10.933	1500	1504	1507	rBV	161291	181730	6.05%	0.726%
18	11.233	1553	1555	1558	rVB	44770	32058	1.07%	0.128%
19	11.333	1568	1572	1575	rBV	908738	803541	26.75%	3.209%
20	11.851	1655	1660	1669	rBV3	152300	207814	6.92%	0.830%
21	12.551	1776	1779	1784	rBV	79052	84052	2.80%	0.336%
22	12.633	1788	1793	1802	rBV2	92801	145618	4.85%	0.582%
23	12.722	1803	1808	1813	rVB2	61723	66117	2.20%	0.264%
24	12.780	1813	1818	1824	rBV2	74997	111181	3.70%	0.444%
25	12.922	1837	1842	1845	rBV	2475958	2481010	82.60%	9.908%
26	13.433	1926	1929	1932	rVB	43317	40484	1.35%	0.162%
27	13.798	1987	1991	1997	rBV2	100472	107436	3.58%	0.429%
28	13.986	2018	2023	2026	rBV	603586	580979	19.34%	2.320%
29	15.033	2198	2201	2203	rBV	27426	37454	1.25%	0.150%
30	15.404	2260	2264	2266	rBV	26582	38178	1.27%	0.152%
31	15.457	2269	2273	2279	rVB	410272	508529	16.93%	2.031%
32	16.345	2419	2424	2432	rBV6	22851	44017	1.47%	0.176%
33	17.421	2602	2607	2613	rVB7	16410	31361	1.04%	0.125%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102717\
Data File : BF099879.D
Acq On : 27 Oct 2017 16:06
Operator : SJ/JU
Sample : I6112-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-MARION26KV-(2-3)

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-BF102317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

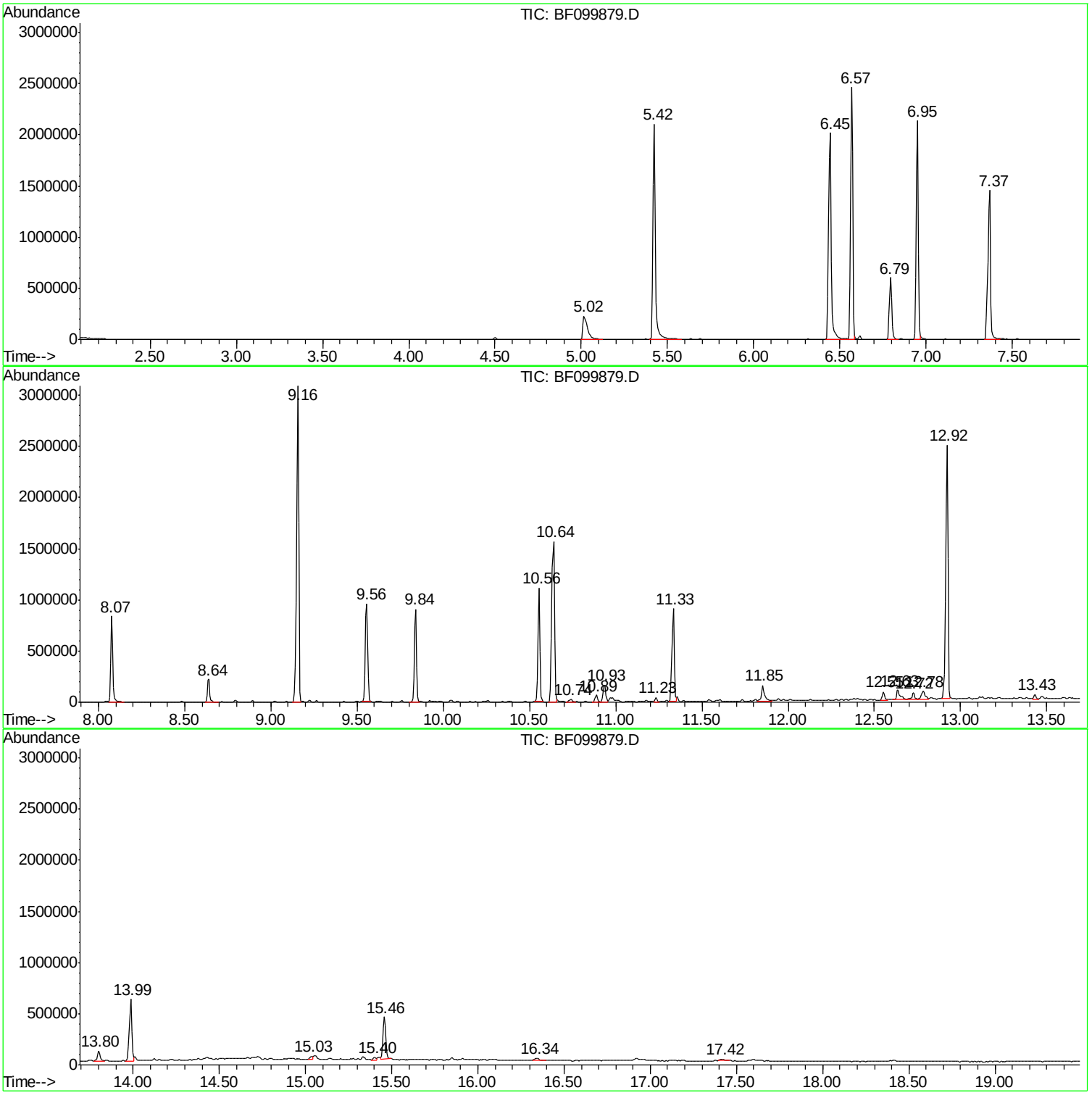
Sum of corrected areas: 25040244

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102717\
Data File : BF099879.D
Acq On : 27 Oct 2017 16:06
Operator : SJ/JU
Sample : I6112-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
2-MARION26KV-(2-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102717\
Data File : BF099879.D
Acq On : 27 Oct 2017 16:06
Operator : SJ/JU
Sample : I6112-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-MARION26KV-(2-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

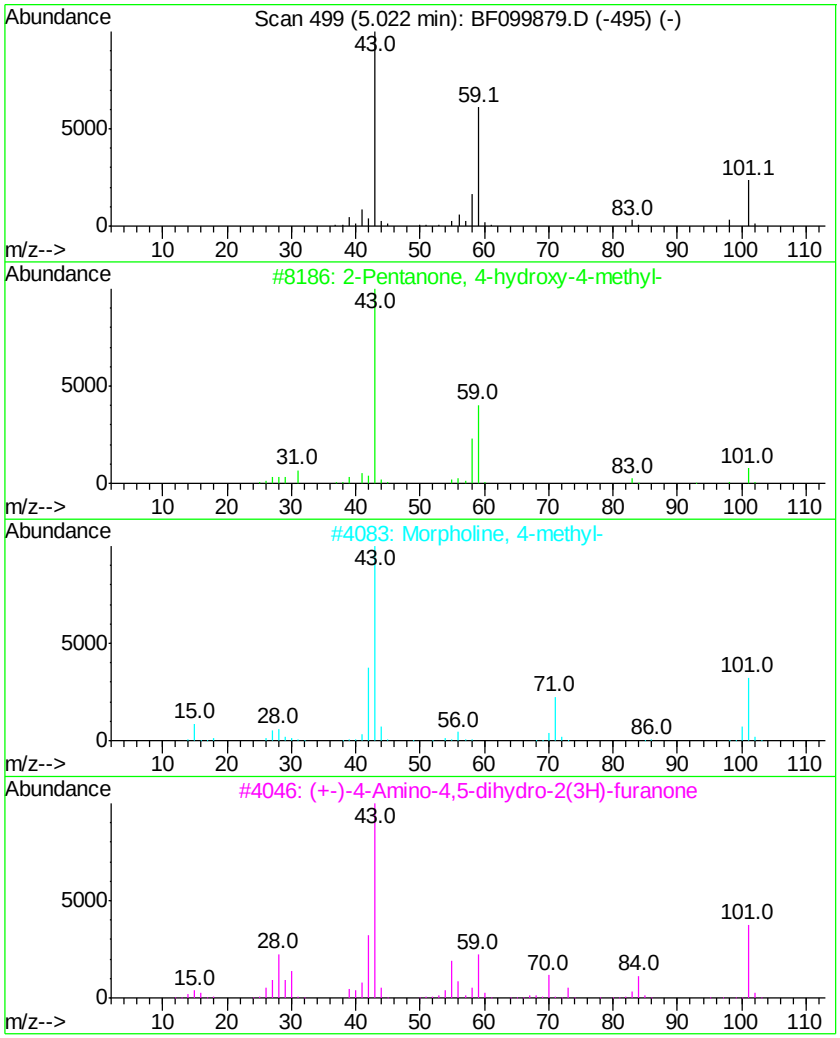
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

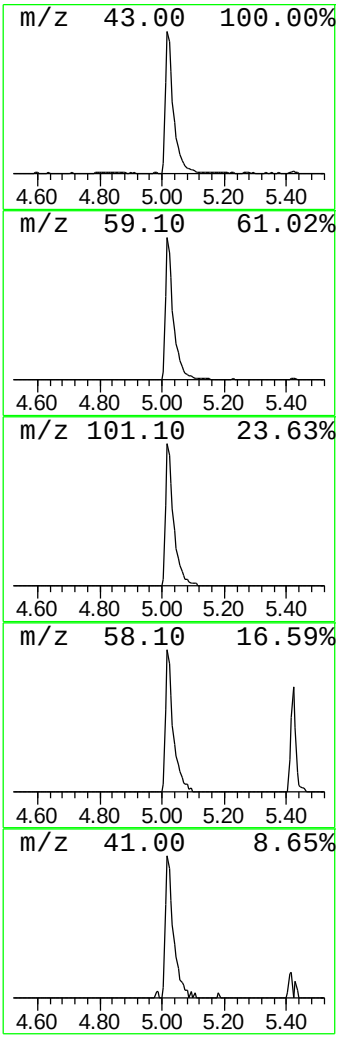
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	15.88 ng	409394	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4	Acetone	58	C3H6O	000067-64-1	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102717\
Data File : BF099879.D
Acq On : 27 Oct 2017 16:06
Operator : SJ/JU
Sample : I6112-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-MARION26KV-(2-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

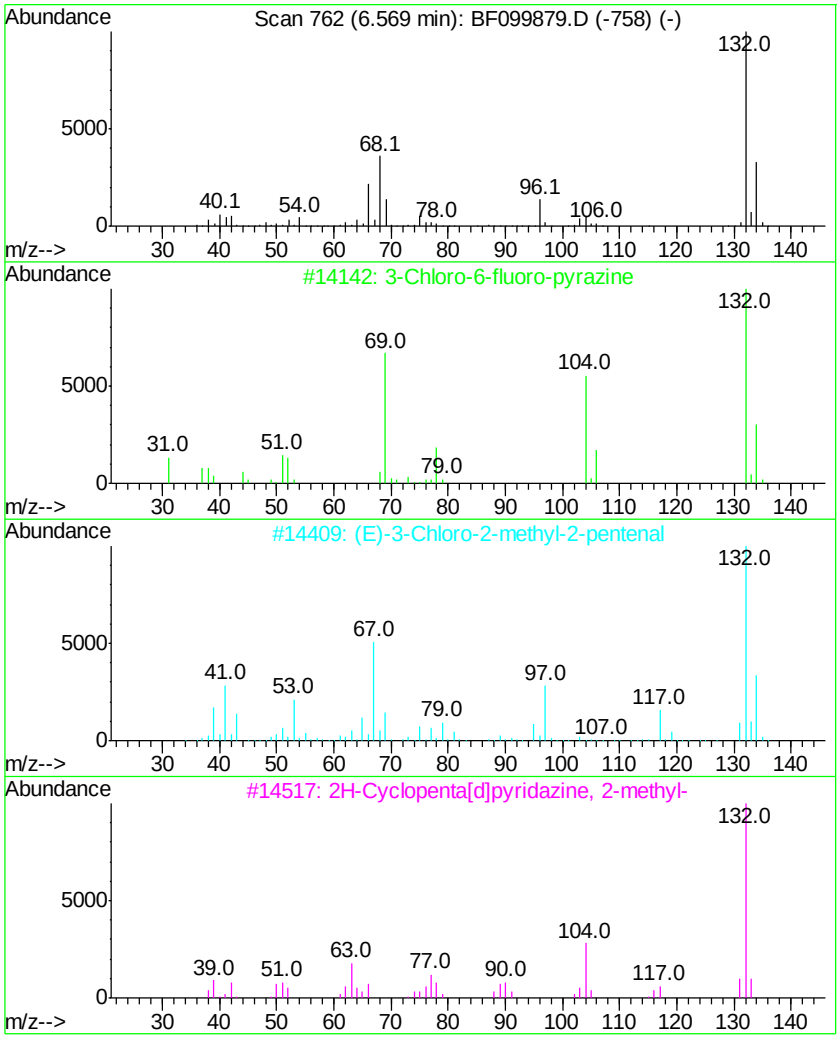
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

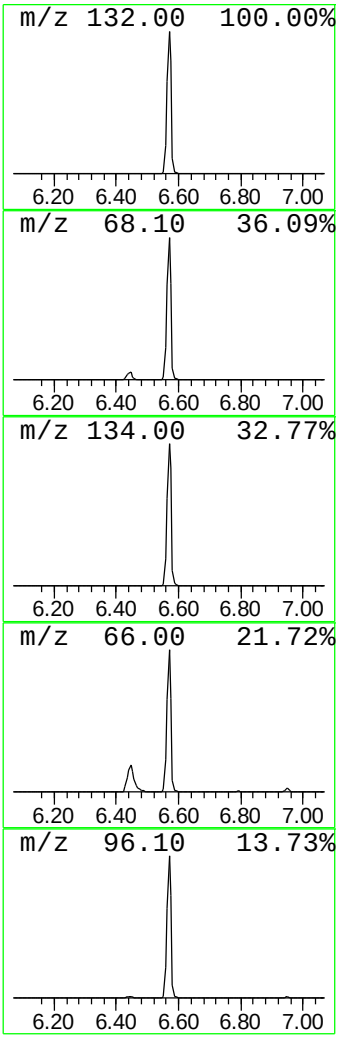
****

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	91.74 ng	2365070	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102717\
Data File : BF099879.D
Acq On : 27 Oct 2017 16:06
Operator : SJ/JU
Sample : I6112-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-MARION26KV-(2-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

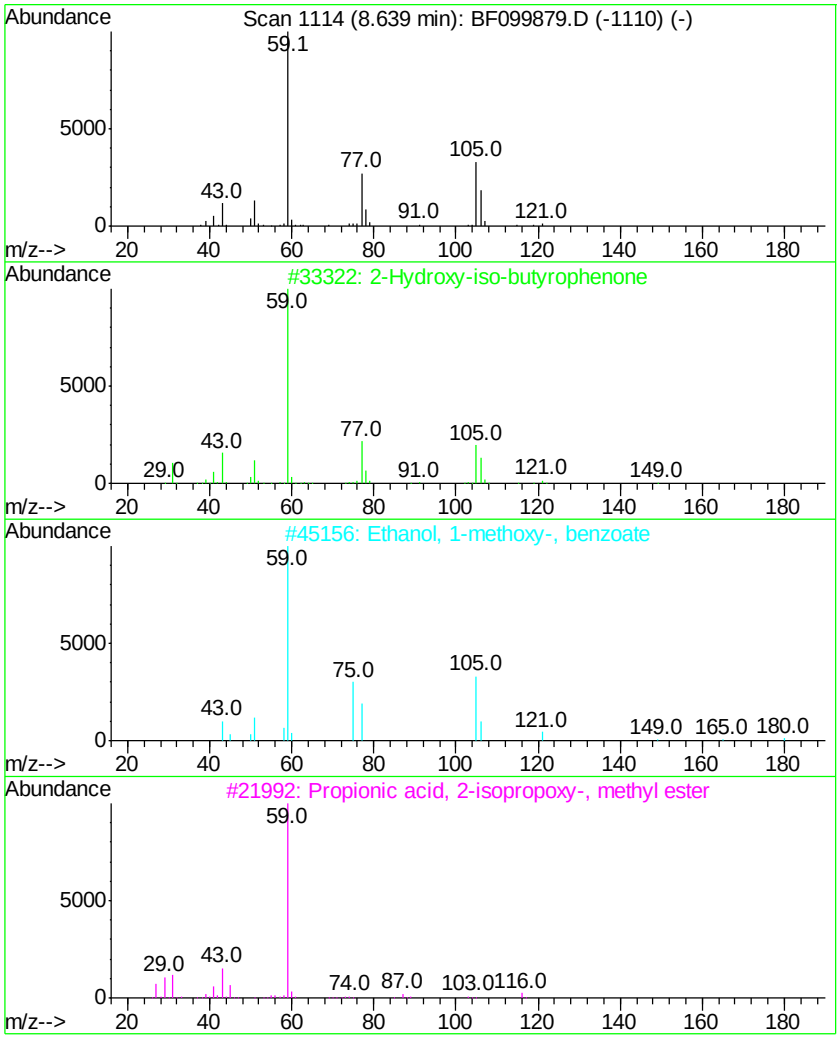
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

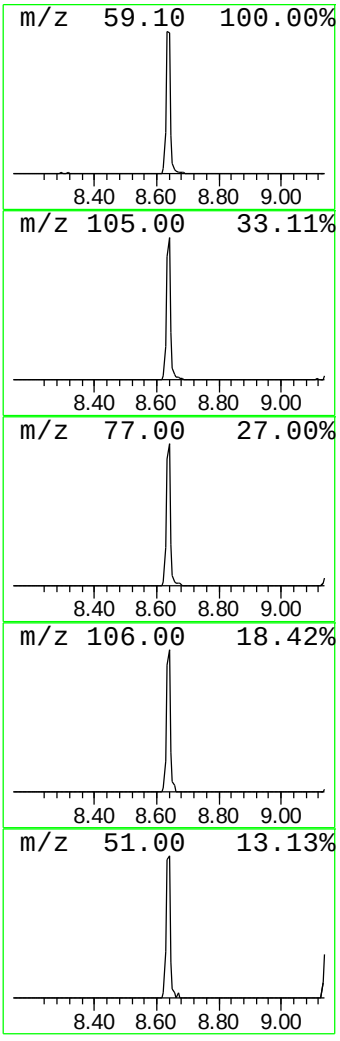
****

Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.64	6.00 ng	222011	Naphthalene-d8	8.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	72
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	50
3	Propionic acid, 2-isopropoxy-, m...	146	C7H14O3	1000151-15-1	9
4	Formamide, N-methyl-	59	C2H5NO	000123-39-7	7
5	.alpha.-(Methylthio)acetamide	105	C3H7NOS	022551-24-2	7





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102717\
Data File : BF099879.D
Acq On : 27 Oct 2017 16:06
Operator : SJ/JU
Sample : I6112-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-MARION26KV-(2-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

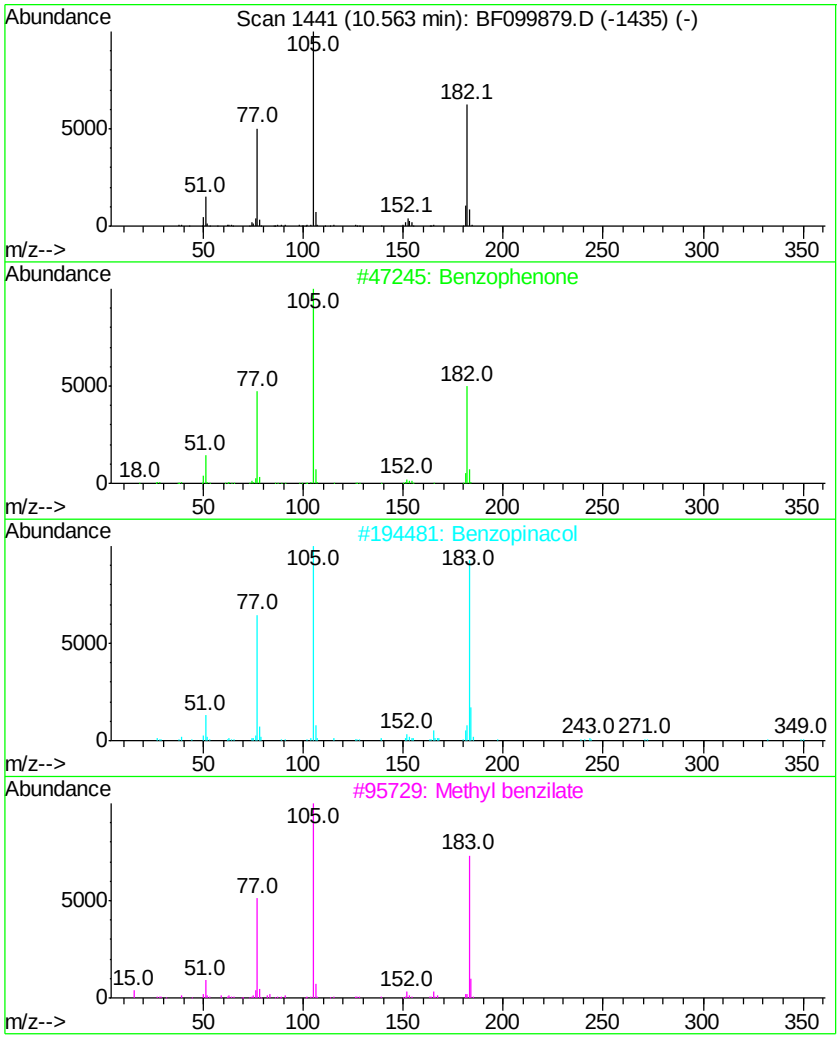
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

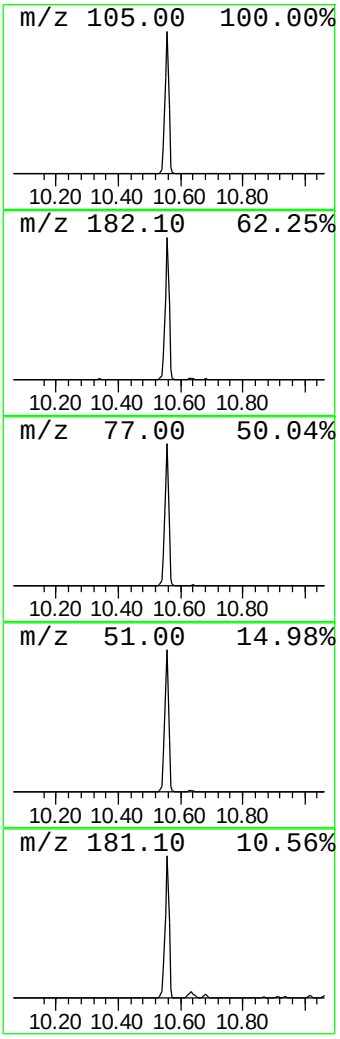
****

Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.56	22.76 ng	930472	Acenaphthene-d10	9.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzopinacol	366	C26H22O2	000464-72-2	50
3	Methyl benzilate	242	C15H14O3	000076-89-1	47
4	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
5	Vinyl benzoate	148	C9H8O2	000769-78-8	43





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102717\
Data File : BF099879.D
Acq On : 27 Oct 2017 16:06
Operator : SJ/JU
Sample : I6112-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-MARION26KV-(2-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

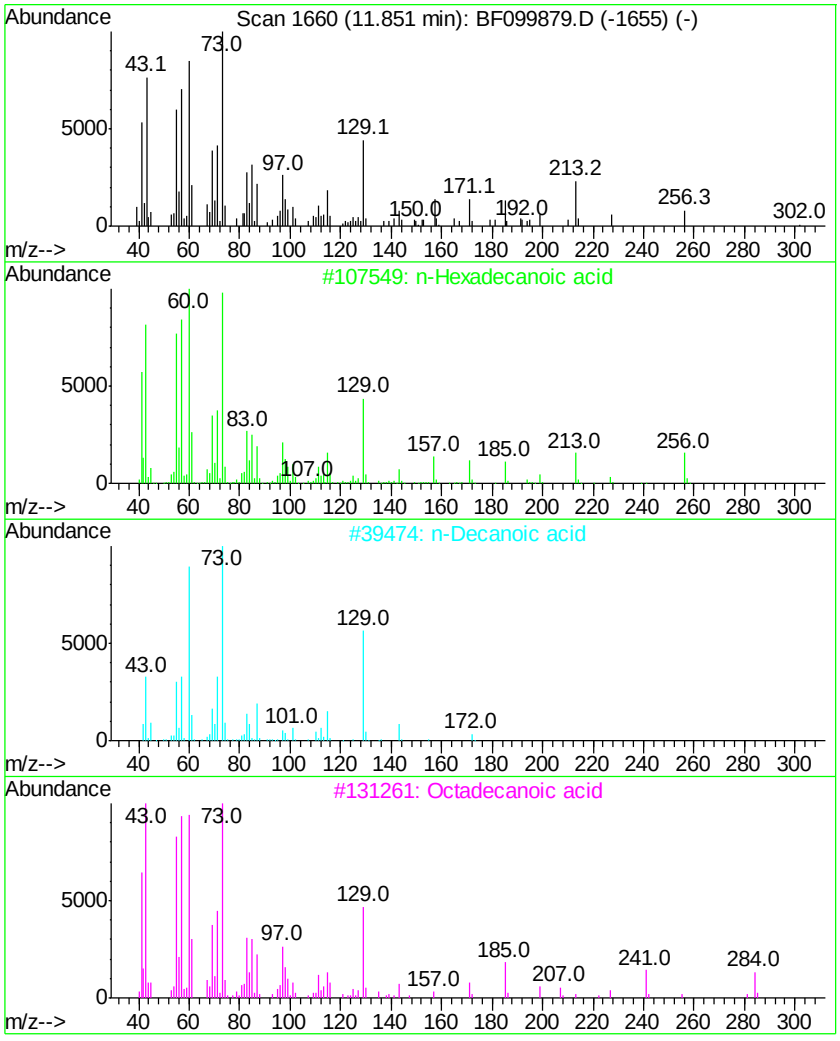
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

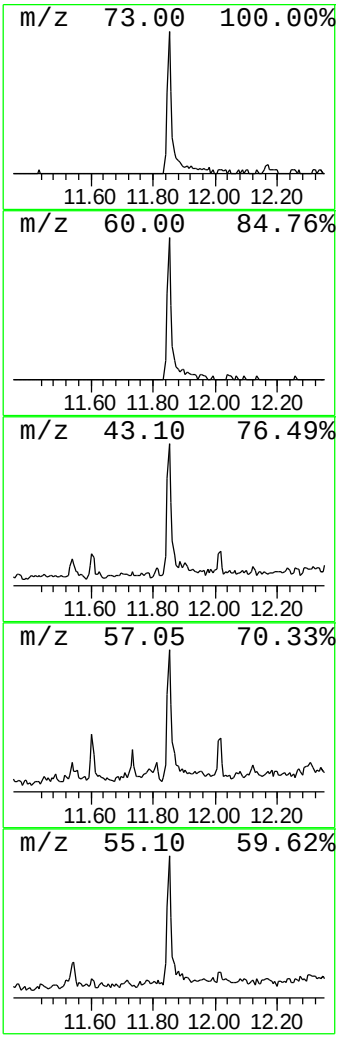
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	5.17 ng	207814	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	n-Decanoic acid	172	C10H20O2	000334-48-5	91
3	Octadecanoic acid	284	C18H36O2	000057-11-4	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	89
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	87





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102717\
Data File : BF099879.D
Acq On : 27 Oct 2017 16:06
Operator : SJ/JU
Sample : I6112-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-MARION26KV-(2-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

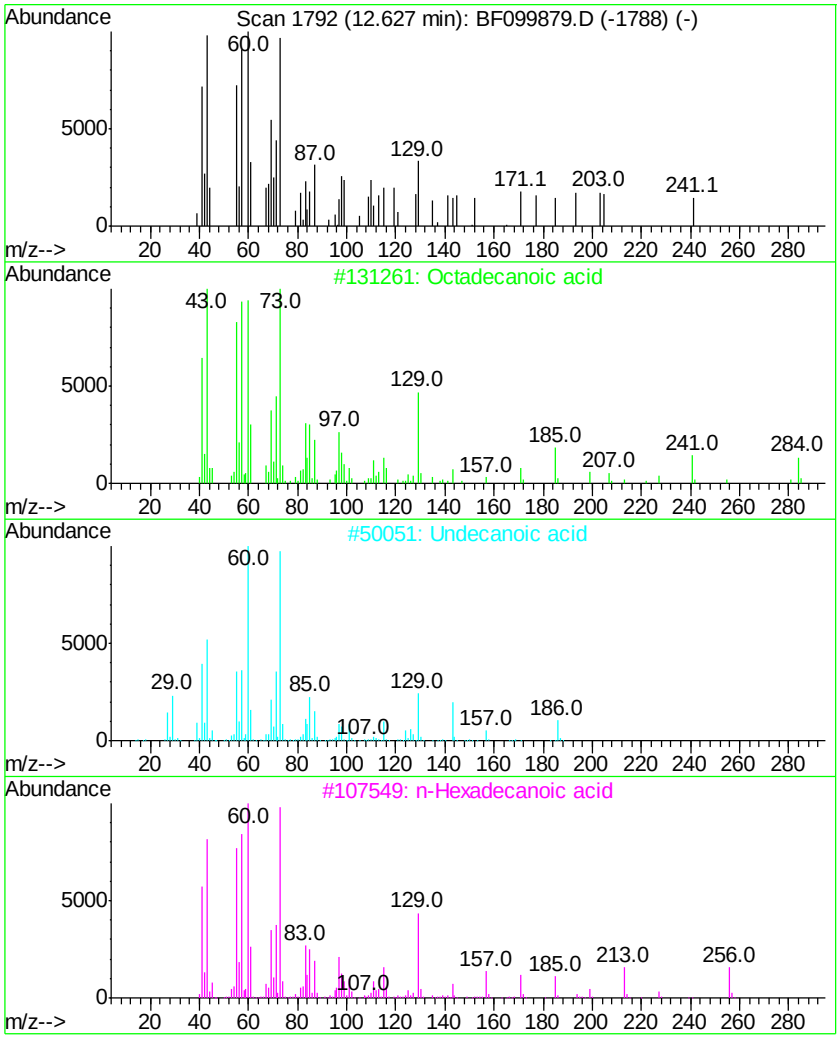
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

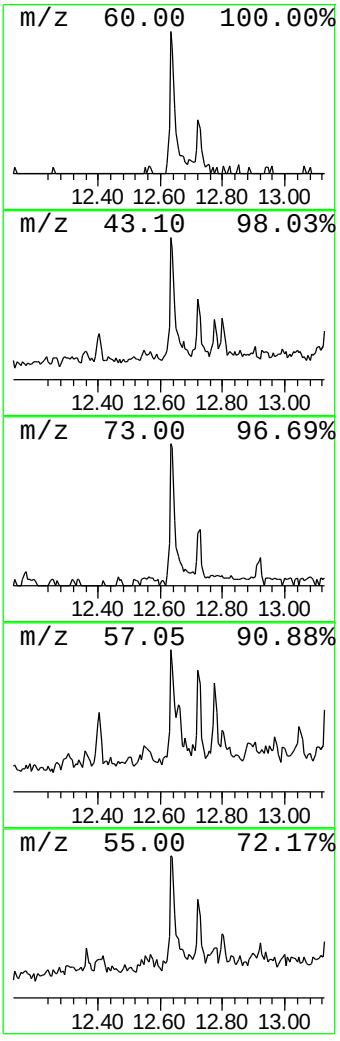
****

Peak Number 9 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	3.62 ng	145618	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2	Undecanoic acid	186	C11H22O2	000112-37-8	91
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102717\
Data File : BF099879.D
Acq On : 27 Oct 2017 16:06
Operator : SJ/JU
Sample : I6112-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-MARION26KV-(2-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

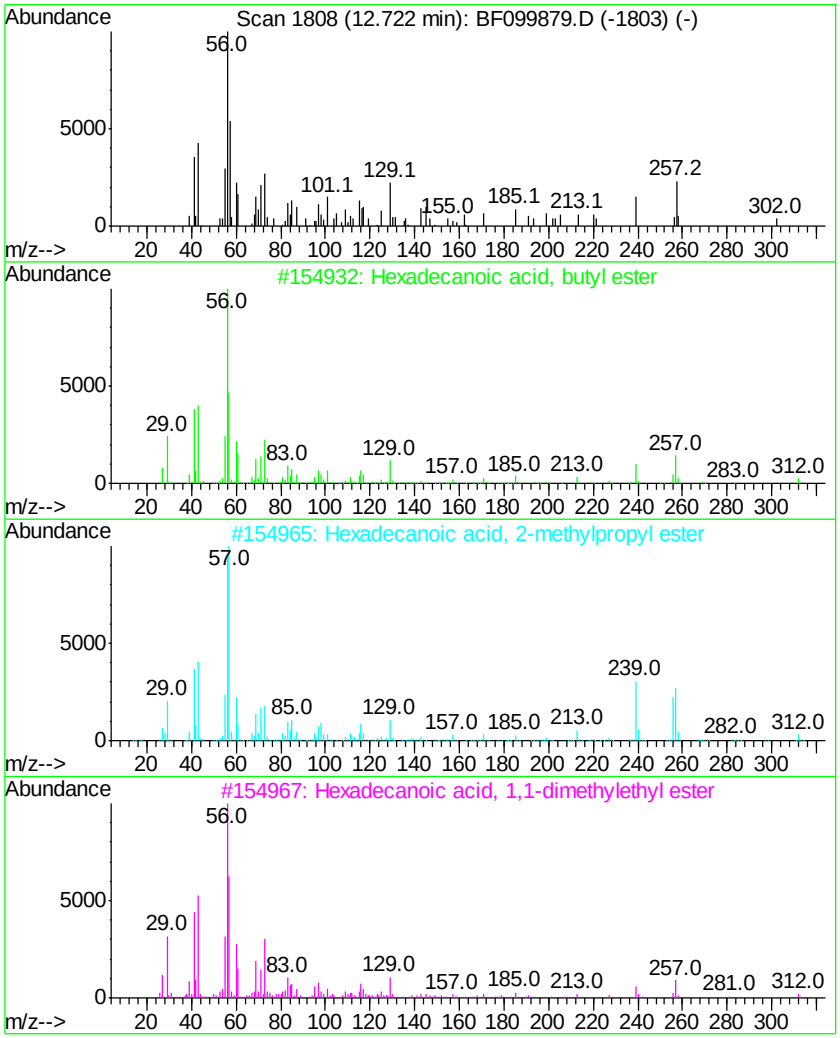
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

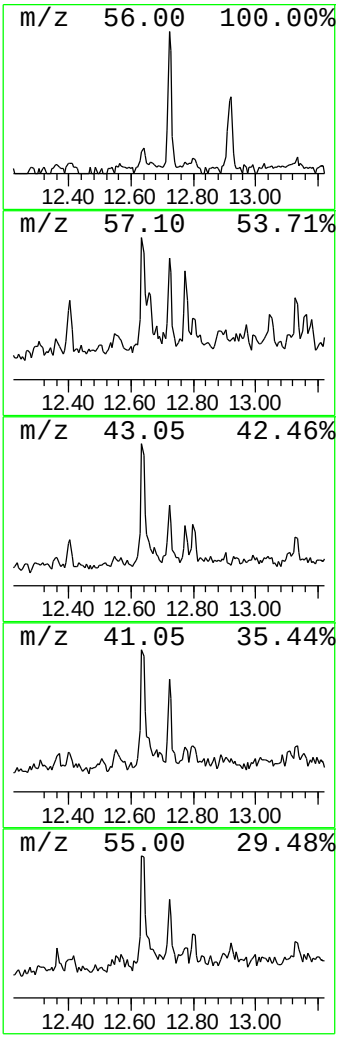
****

Peak Number 10 Hexadecanoic acid, butyl ester Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	2.28 ng	66117	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	64
2	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	53
3	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	53
4	Cyclopentanone, 2,2-dimethyl-	112	C7H12O	004541-32-6	30
5	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	30





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102717\
Data File : BF099879.D
Acq On : 27 Oct 2017 16:06
Operator : SJ/JU
Sample : I6112-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-MARION26KV-(2-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

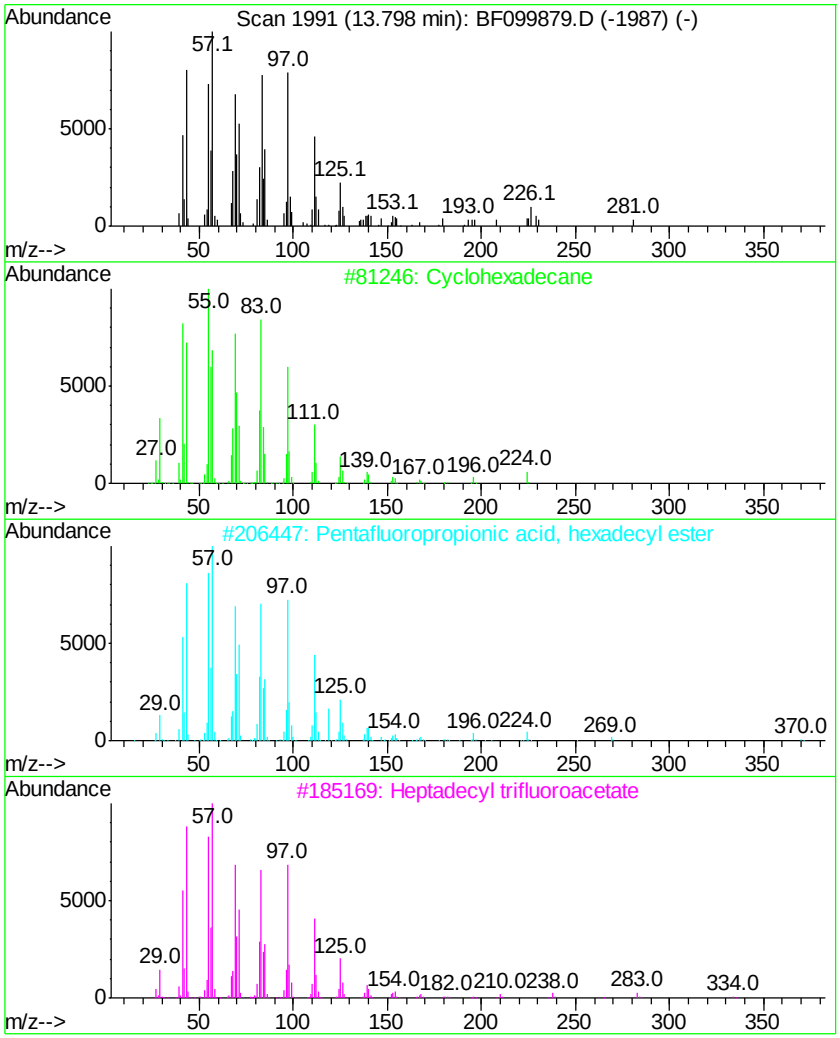
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

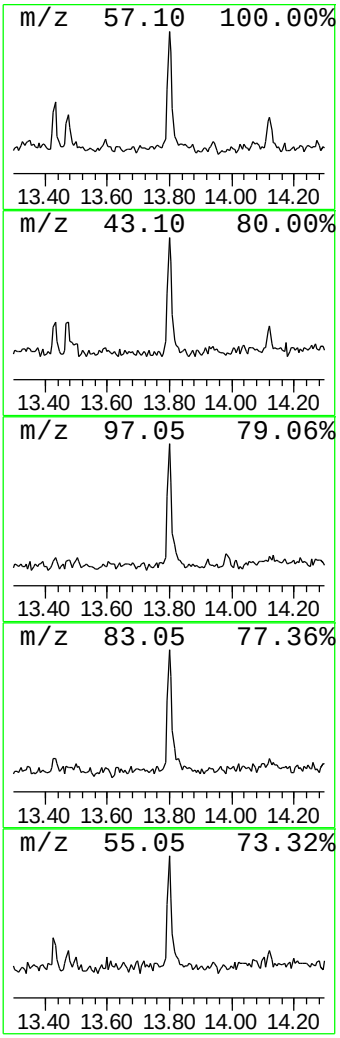
****

Peak Number 12 Cyclohexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	3.70 ng	107436	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	95
2	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	93
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102717\
Data File : BF099879.D
Acq On : 27 Oct 2017 16:06
Operator : SJ/JU
Sample : I6112-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-MARION26KV-(2-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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
2-Pentanone, 4-hy...	5.02	15.9	ng	409394	1	6.79	515586	20.0
unknown6.57	6.57	91.7	ng	2365070	1	6.79	515586	20.0
2-Hydroxy-iso-but...	8.64	6.0	ng	222011	2	8.07	740348	20.0
Benzophenone	10.56	22.8	ng	930472	3	9.84	817659	20.0
n-Hexadecanoic acid	11.85	5.2	ng	207814	4	11.33	803541	20.0
Octadecanoic acid	12.63	3.6	ng	145618	4	11.33	803541	20.0
Hexadecanoic acid...	12.72	2.3	ng	66117	5	13.99	580979	20.0
Cyclohexadecane	13.80	3.7	ng	107436	5	13.99	580979	20.0