LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102745.D
Acq On : 5 Feb 2018 18:33
Operator : SJ/JU
Sample : J1456-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SA-ST-LATERAL-LINE-2-SW@4

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	2.181	10	16	23	rVB	474768	625673	11.67%	1.349%
2	5.122	512	516	526	rVB	149281	205889	3.84%	0.444%
3	5.498	575	580	583	rBV	4663981	5200037	97.02%	11.211%
4	6.510	745	752	756	rBV2	4223616	5359812	100.00%	11.556%
5	6.651	771	776	779	rBV	5031151	5043804	94.10%	10.874%
6	6.881	811	815	818	rBV	1669677	1348782	25.16%	2.908%
7	7.040	837	842	845	rBV	3850037	3584184	66.87%	7.727%
8	7.445	901	911	914	rBV	3200220	3310747	61.77%	7.138%
9	7.628	938	942	944	rBV	85163	72973	1.36%	0.157%
10	8.163	1028	1033	1036	rBV	2201707	1792443	33.44%	3.864%
11	9.239	1210	1216	1219	rBV	4859585	4363389	81.41%	9.407%
12	9.310	1225	1228	1231	rBV	98222	91086	1.70%	0.196%
13	9.339	1231	1233	1244	rVB3	27526	60040	1.12%	0.129%
14	9.628	1278	1282	1285	rBV	734723	564349	10.53%	1.217%
15	9.816	1311	1314	1316	rBV2	69229	81879	1.53%	0.177%
16	9.845	1316	1319	1322	rVB	277879	221113	4.13%	0.477%
17	9.916	1327	1331	1335	rVB2	1976351	1822213	34.00%	3.929%
18	10.075	1353	1358	1361	rBV2	37724	54777	1.02%	0.118%
19	10.163	1370	1373	1377	rBV3	54827	58336	1.09%	0.126%
20	10.345	1401	1404	1407	rVB	324502	246150	4.59%	0.531%
21	10.563	1436	1441	1444	rBV	87447	110733	2.07%	0.239%
22	10.704	1459	1465	1469	rBV	2736408	2835487	52.90%	6.113%
23	10.816	1481	1484	1493	rVB	270938	266121	4.97%	0.574%
24	10.969	1504	1510	1513	rVB	64906	64789	1.21%	0.140%
25	11.263	1557	1560	1563	rBV	114764	93028	1.74%	0.201%
26	11.404	1580	1584	1587	rBV	1838153	1536427	28.67%	3.312%
27	11.927	1668	1673	1681	rBV	618233	639705	11.94%	1.379%
28	12.710	1802	1806	1816	rBV	234833	264168	4.93%	0.570%
29	12.992	1849	1854	1857	rBV	3285504	3142215	58.63%	6.774%
30	13.463	1929	1934	1939	rVB2	58219	65780	1.23%	0.142%
31	13.874	2000	2004	2013	rBV	388607	368685	6.88%	0.795%
32	14.039	2028	2032	2036	rBV	1174748	1086525	20.27%	2.343%
33	14.510	2108	2112	2115	rBV2	49242	54984	1.03%	0.119%
34	14.798	2157	2161	2171	rBV	471214	615217	11.48%	1.326%

LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102745.D
Acq On : 5 Feb 2018 18:33
Operator : SJ/JU
Sample : J1456-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SA-ST-LATERAL-LINE-2-SW@4

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	15.521	2278	2284	2294	rBV	759438	1063500	19.84%	2.293%
36	16.039	2368	2372	2378	rVB5	39985	68061	1.27%	0.147%

Sum of corrected areas: 46383101

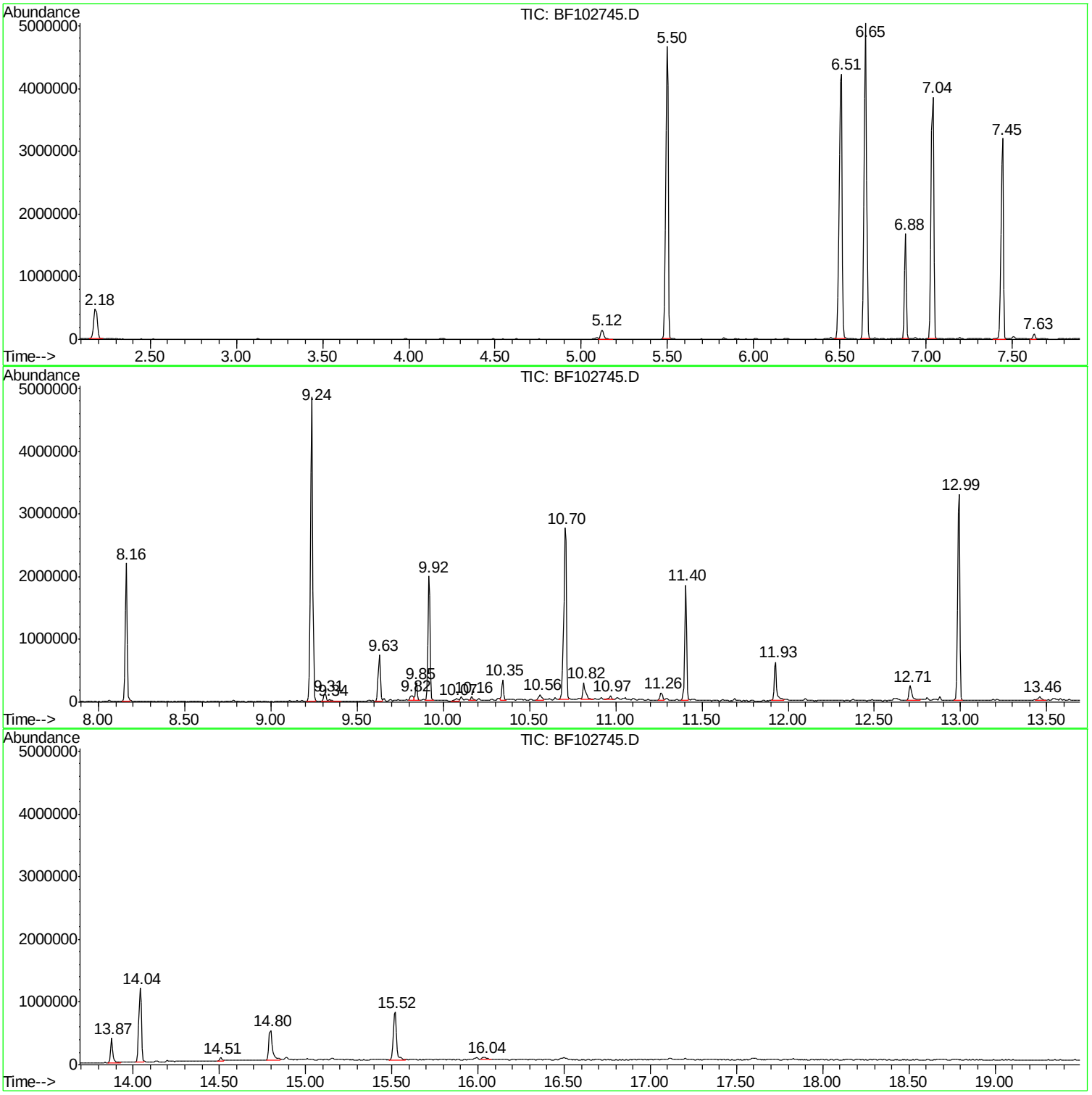
LSC Report - Integrated Chromatogram

Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102745.D
Acq On : 5 Feb 2018 18:33
Operator : SJ/JU
Sample : J1456-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-ST-LATERAL-LINE-2-SW@4

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



Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102745.D
Acq On : 5 Feb 2018 18:33
Operator : SJ/JU
Sample : J1456-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-ST-LATERAL-LINE-2-SW@4

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

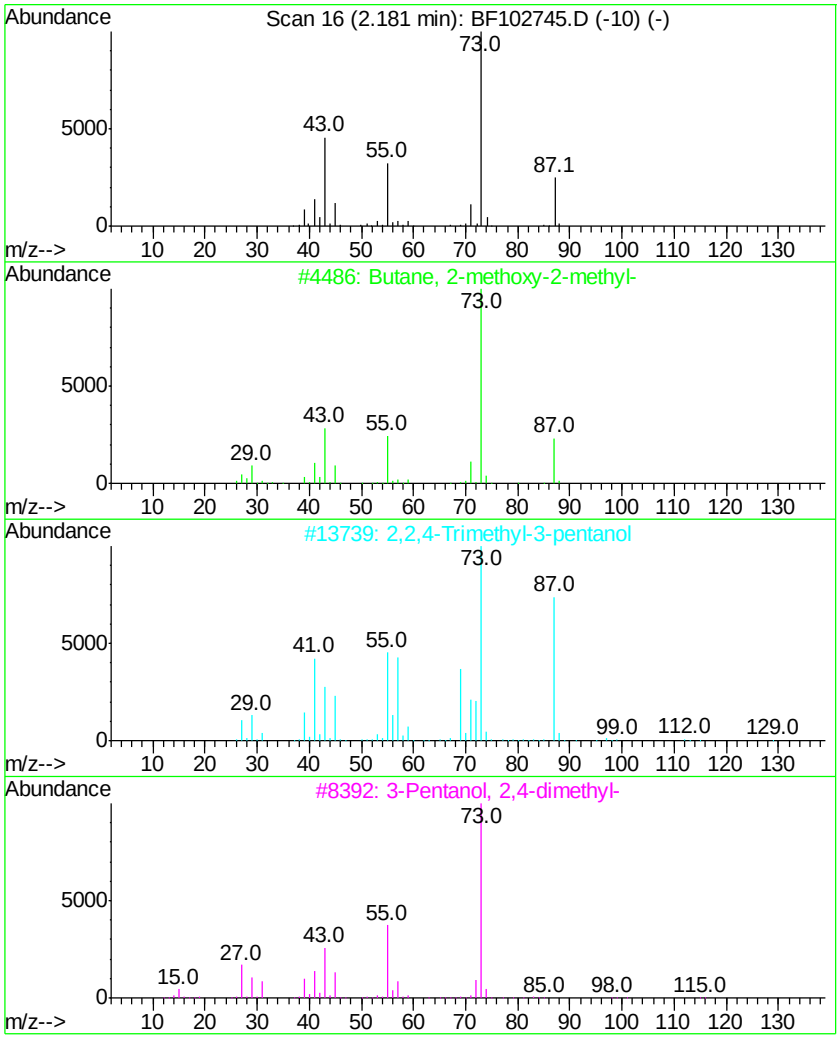
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

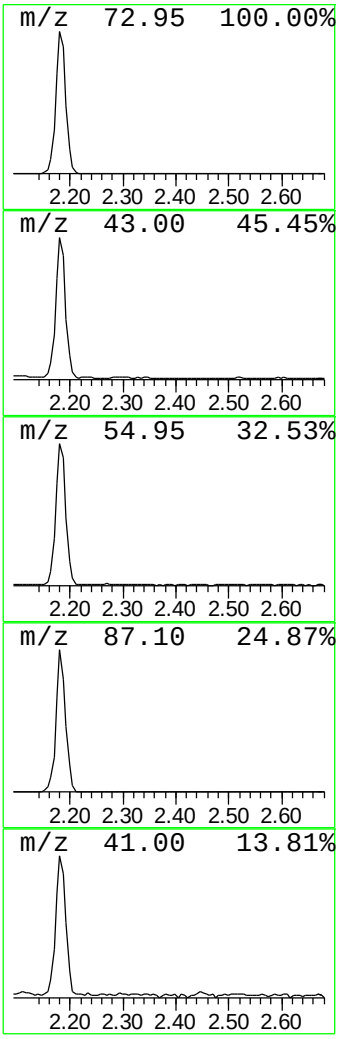
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	9.28 ng	625673	1,4-Dichlorobenzene-d4	6.88

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	40
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





Library Search Compound Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102745.D
Acq On : 5 Feb 2018 18:33
Operator : SJ/JU
Sample : J1456-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-ST-LATERAL-LINE-2-SW@4

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

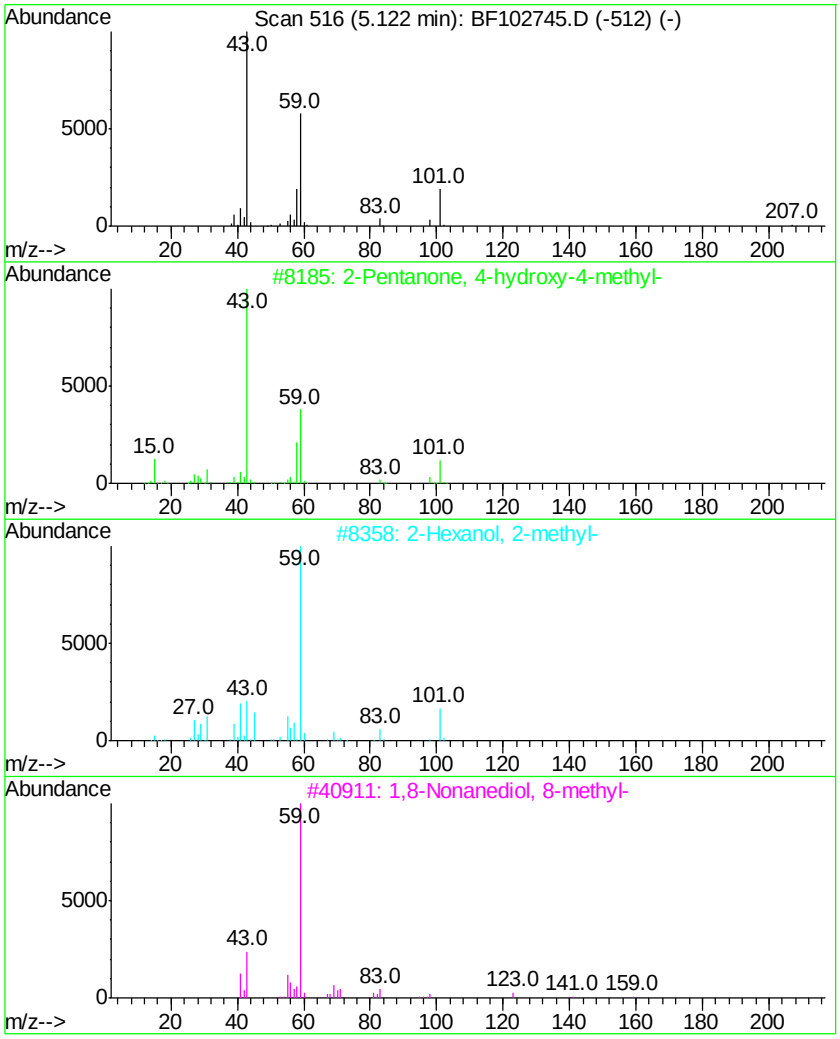
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

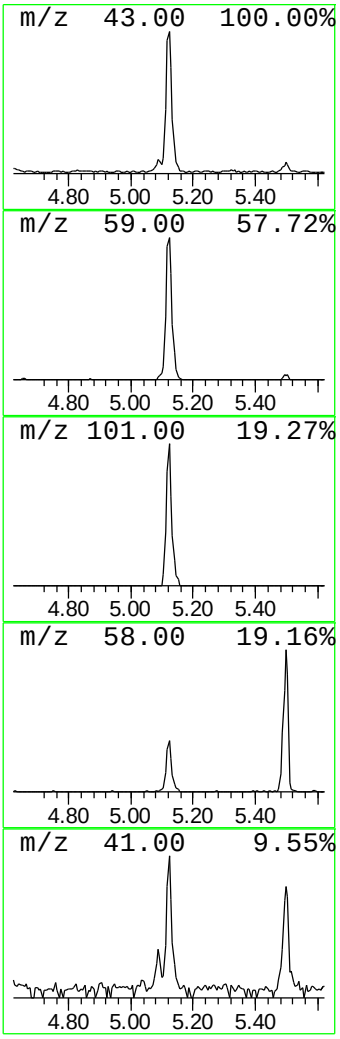
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	3.05 ng	205889	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
4	2-Nonanone	142	C9H18O	000821-55-6	17
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102745.D
Acq On : 5 Feb 2018 18:33
Operator : SJ/JU
Sample : J1456-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SA-ST-LATERAL-LINE-2-SW@4

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

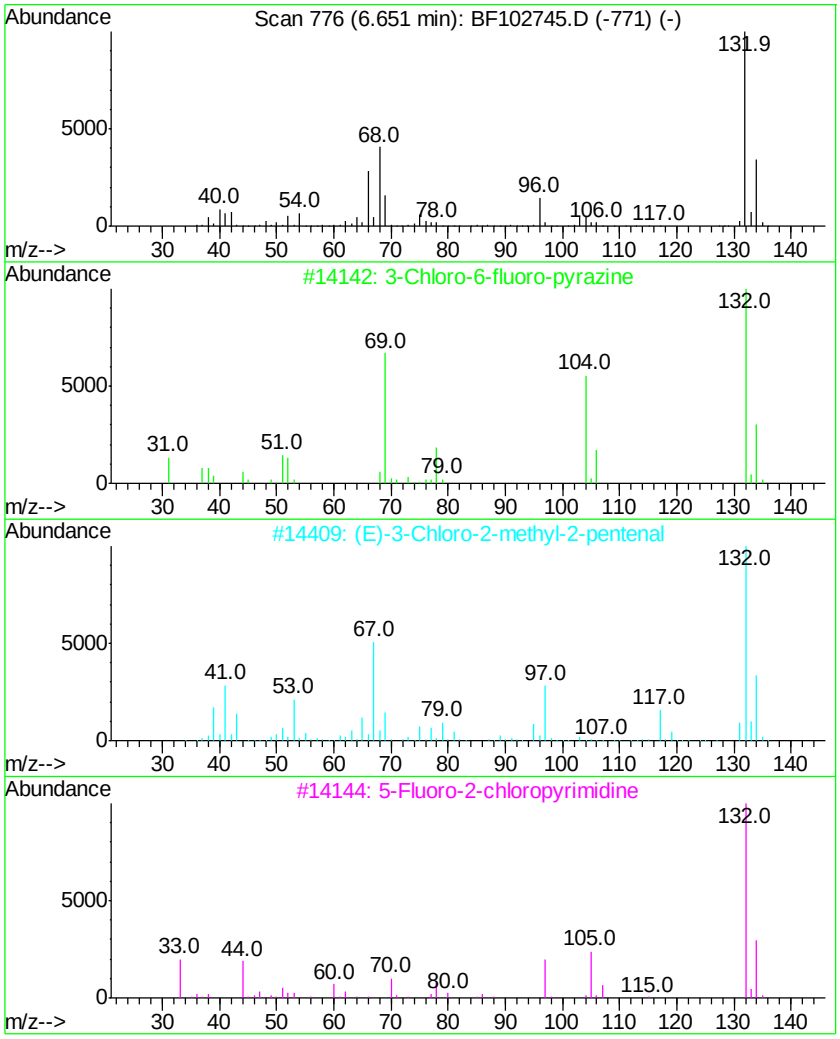
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

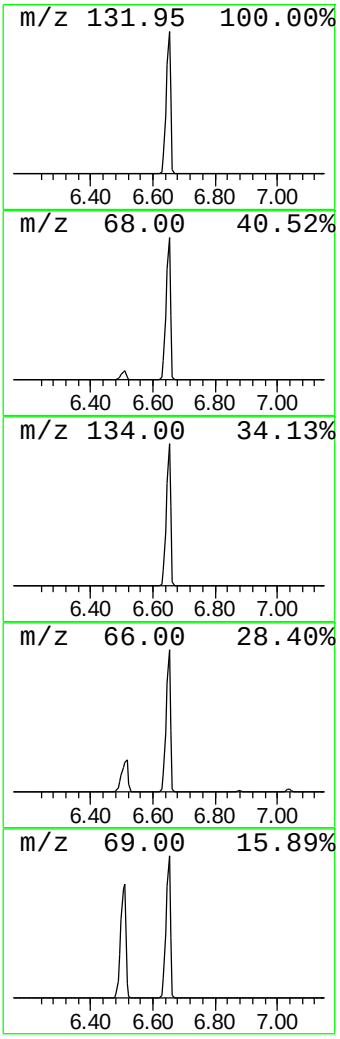
****

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	74.79 ng	5043800	1,4-Dichlorobenzene-d4	6.88

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-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Library Search Compound Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
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Acq On : 5 Feb 2018 18:33
Operator : SJ/JU
Sample : J1456-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-ST-LATERAL-LINE-2-SW@4

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

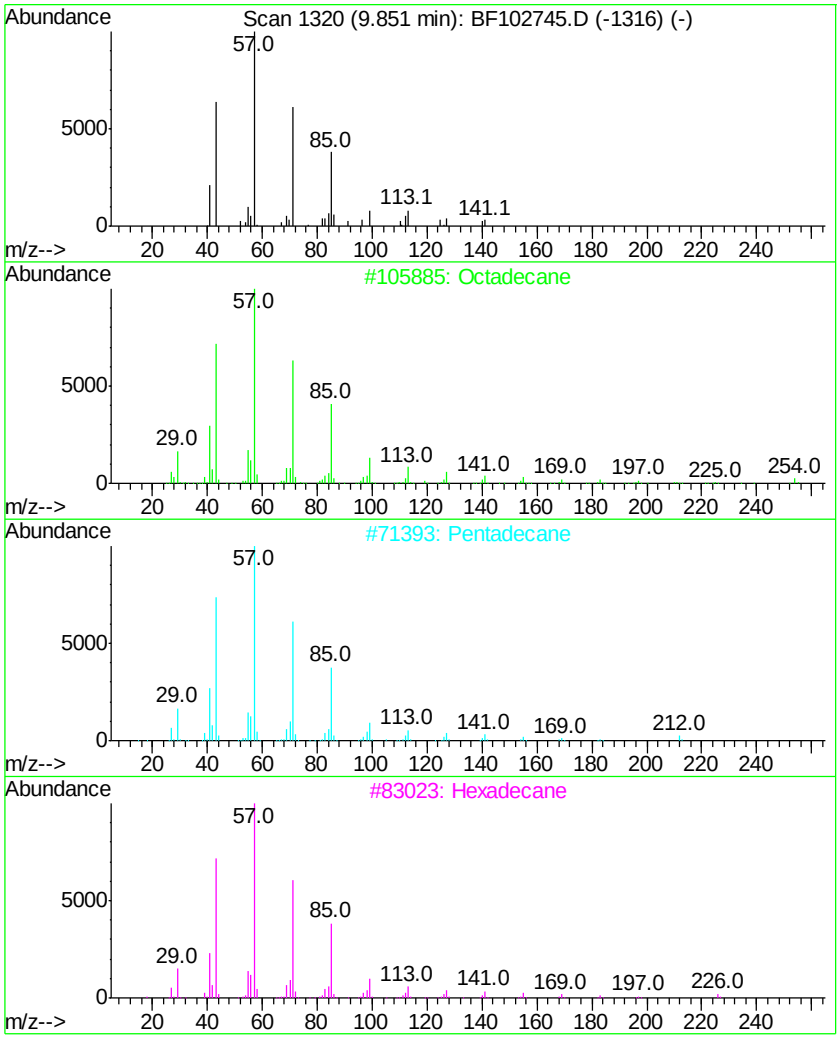
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

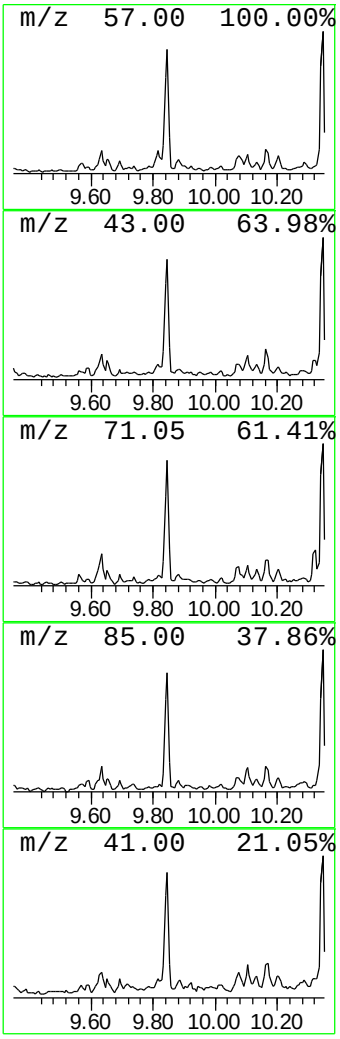
****

Peak Number 5 Octadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.85	2.43 ng	221113	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	83
2	Pentadecane	212	C15H32	000629-62-9	83
3	Hexadecane	226	C16H34	000544-76-3	83
4	Undecane, 5-ethyl-	184	C13H28	017453-94-0	78
5	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	72





Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102745.D
Acq On : 5 Feb 2018 18:33
Operator : SJ/JU
Sample : J1456-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-ST-LATERAL-LINE-2-SW@4

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

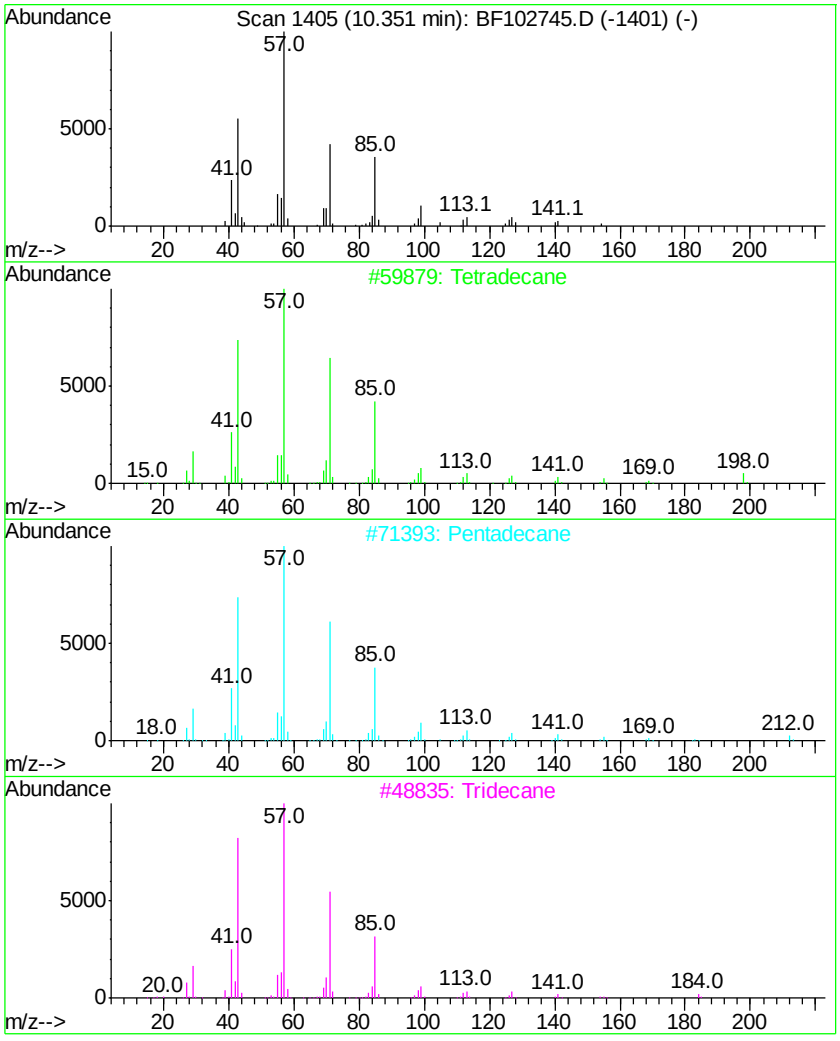
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

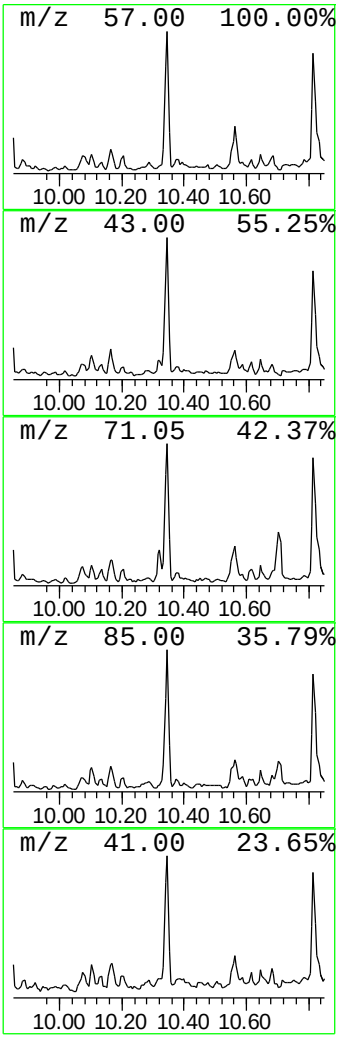
****

Peak Number 6 Tetradecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.35	2.70 ng	246150	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	90
2	Pentadecane	212	C15H32	000629-62-9	90
3	Tridecane	184	C13H28	000629-50-5	90
4	Octadecane	254	C18H38	000593-45-3	90
5	Hexadecane	226	C16H34	000544-76-3	87





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Sample : J1456-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-ST-LATERAL-LINE-2-SW@4

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

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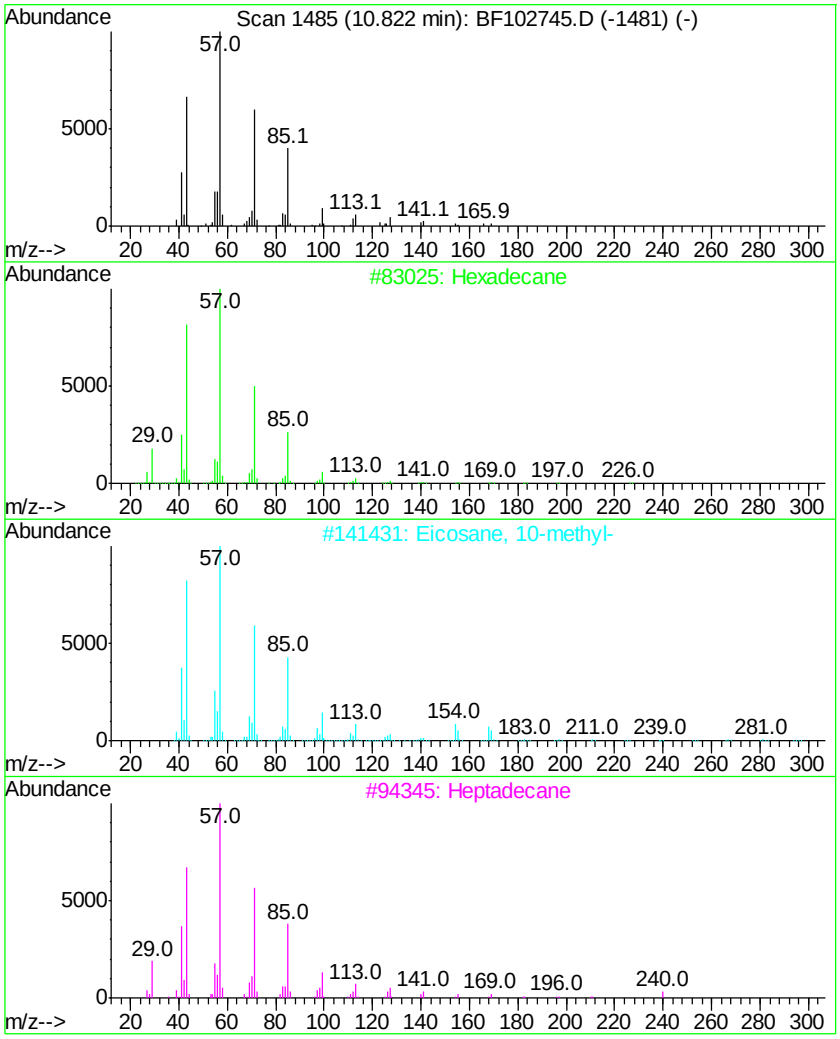
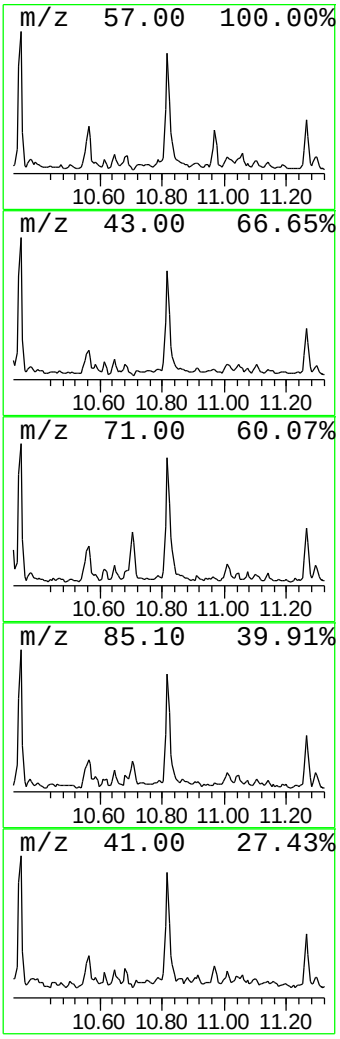
Peak Number 7 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	3.46 ng	266121	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
3	Heptadecane	240	C17H36	000629-78-7	90
4	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	86
5	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	83





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : SA-ST-LATERAL-LINE-2-SW@4

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

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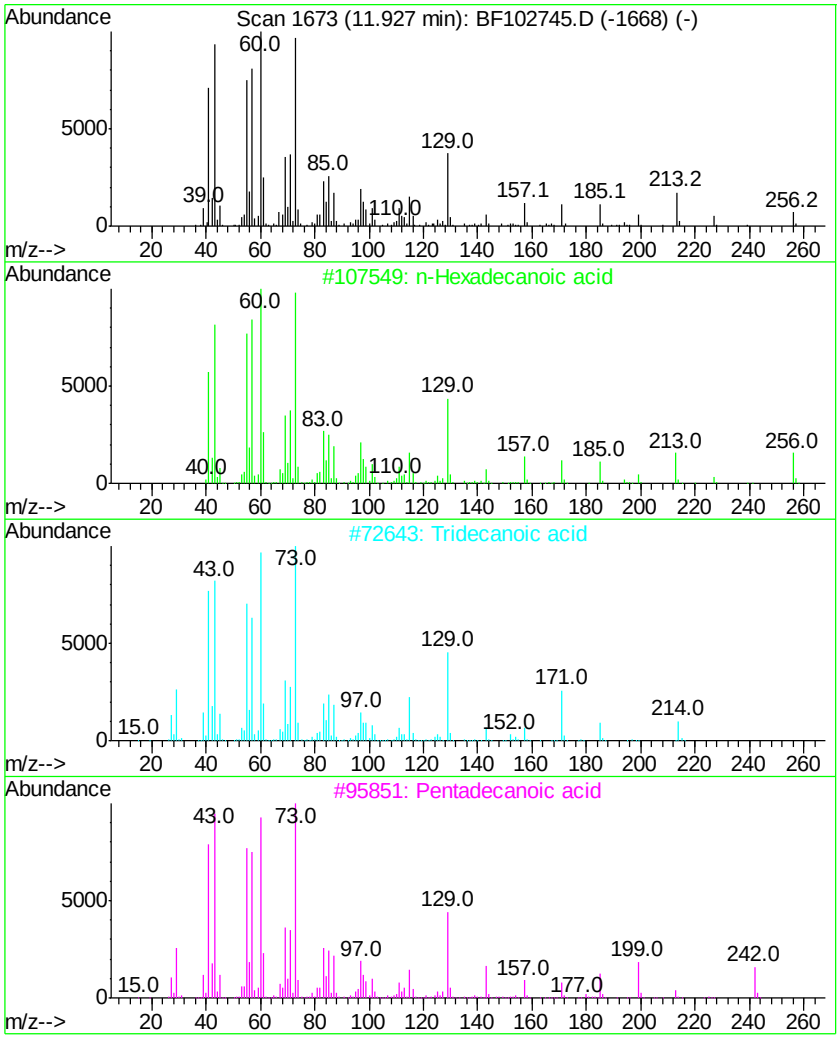
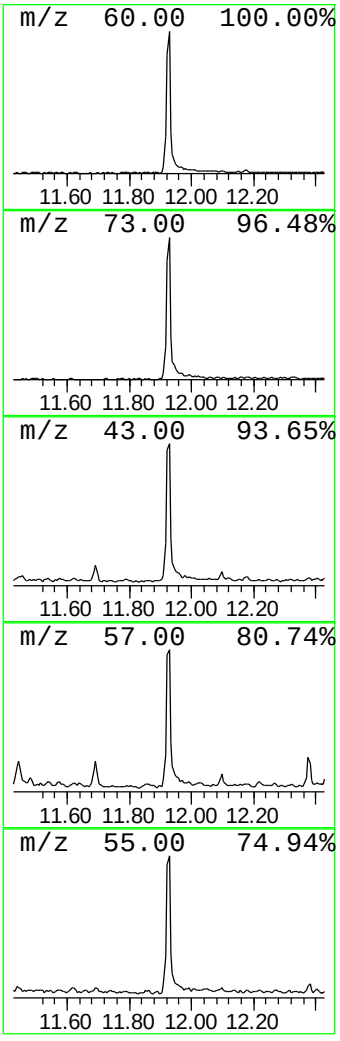
Peak Number 8 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	8.33 ng	639705	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	Dodecanoic acid	200	C12H24O2	000143-07-7	76





Library Search Compound Report

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Instrument :
BNA_F
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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

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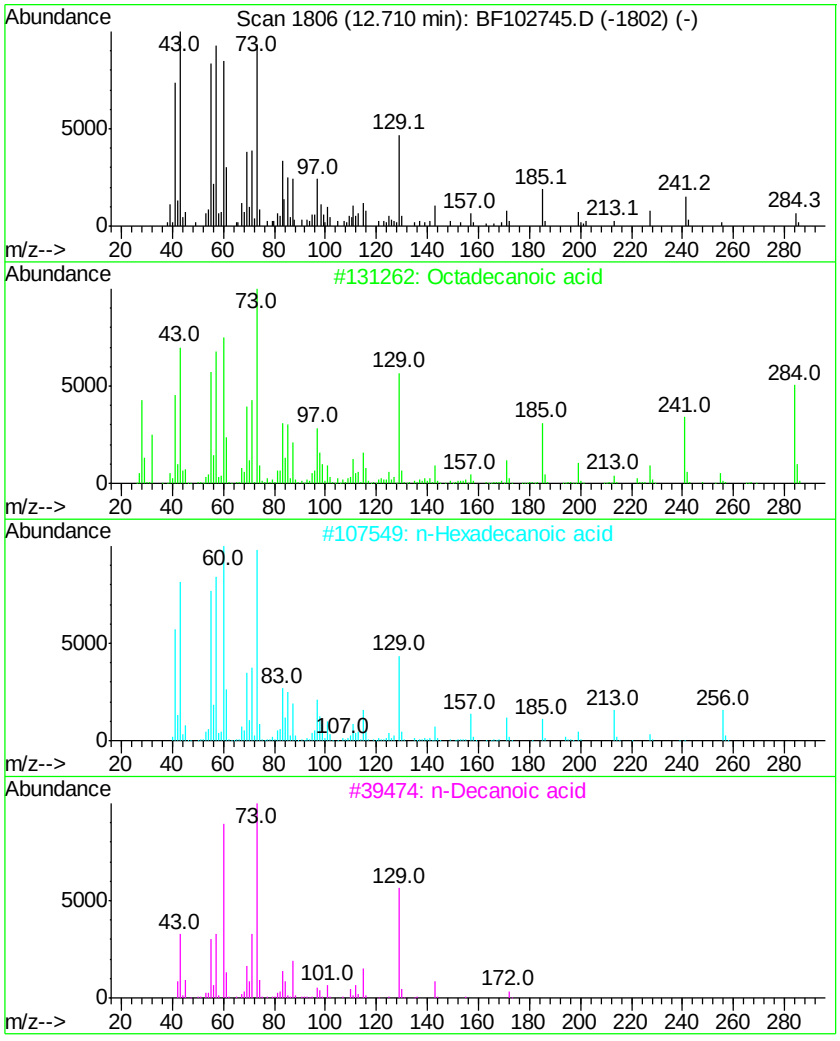
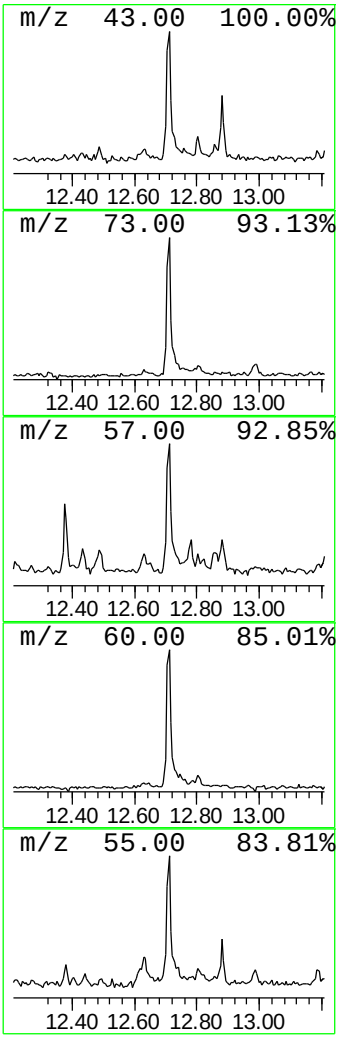
Peak Number 9 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	3.44 ng	264168	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3	n-Decanoic acid	172	C10H20O2	000334-48-5	89
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
5	Undecanoic acid	186	C11H22O2	000112-37-8	68





Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102745.D
Acq On : 5 Feb 2018 18:33
Operator : SJ/JU
Sample : J1456-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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

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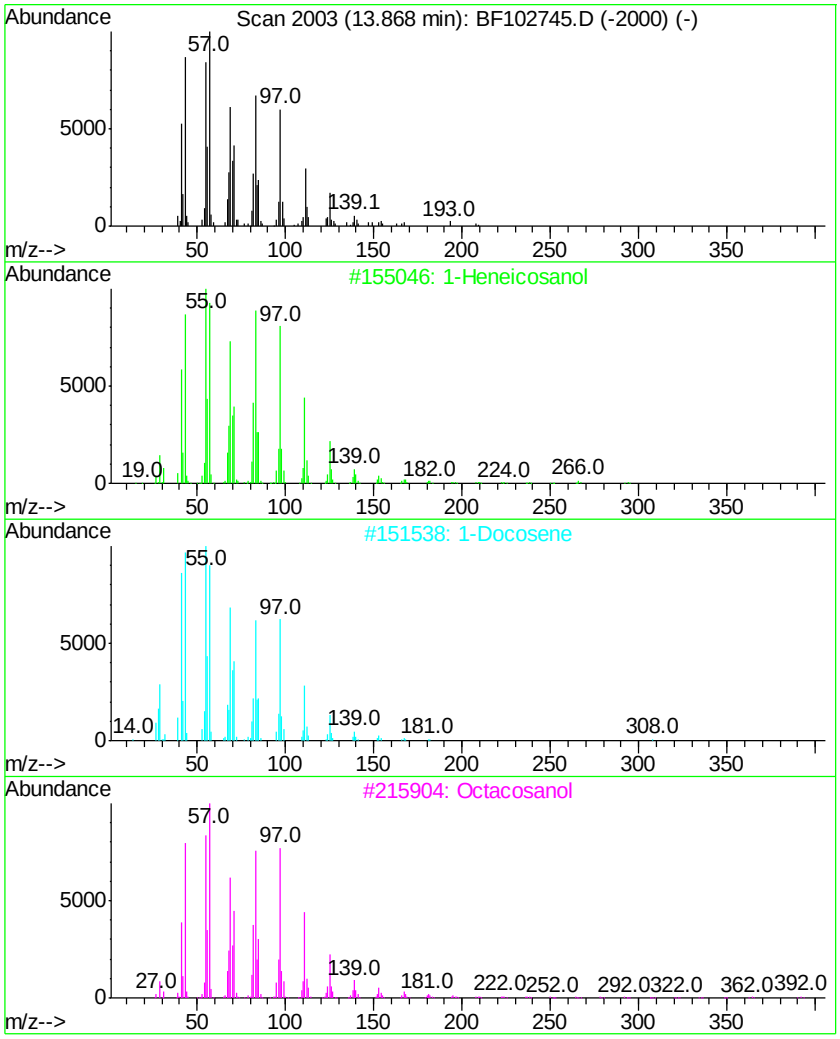
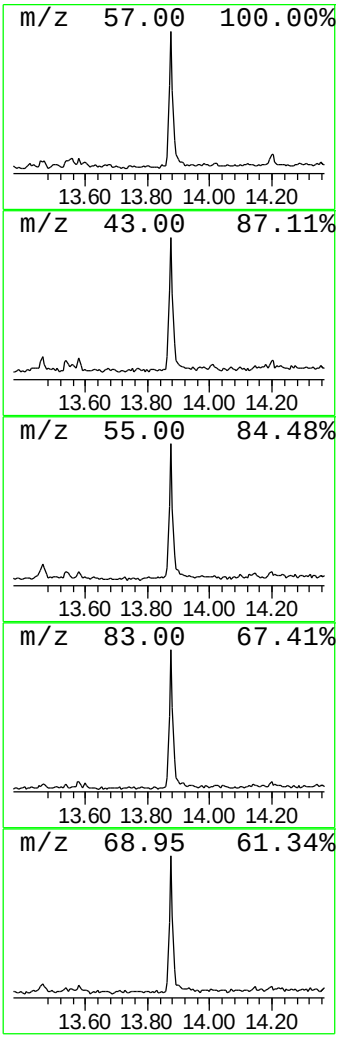
Peak Number 10 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	6.79 ng	368685	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	1-Docosene	308	C22H44	001599-67-3	94
3	Octacosanol	410	C28H58O	000557-61-9	91
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5	Behenic alcohol	326	C22H46O	000661-19-8	91





Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102745.D
Acq On : 5 Feb 2018 18:33
Operator : SJ/JU
Sample : J1456-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-ST-LATERAL-LINE-2-SW@4

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

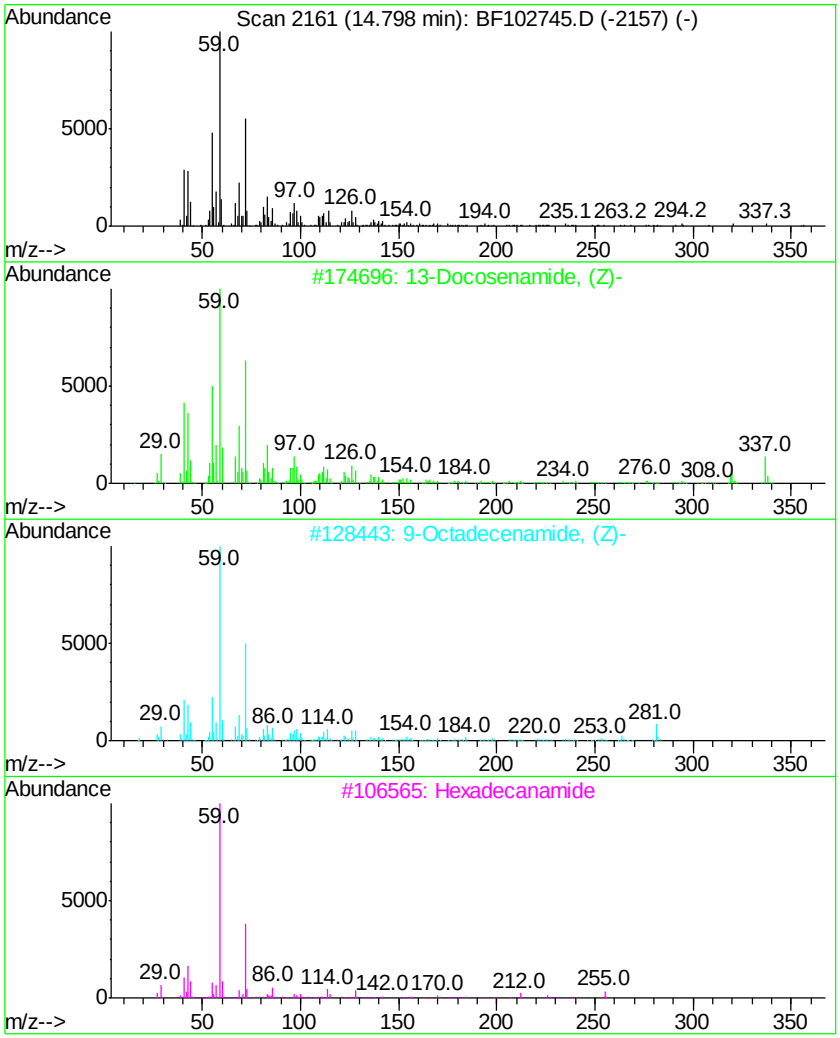
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

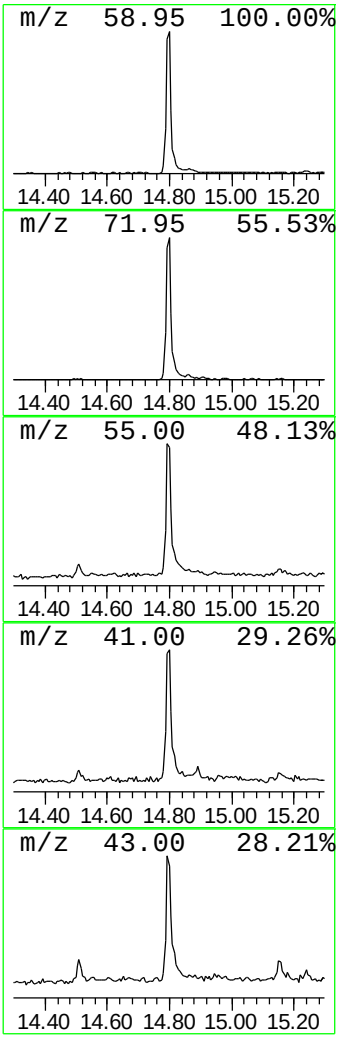
****

Peak Number 11 13-Docosenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	11.57 ng	615217	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
3	Hexadecanamide	255	C16H33NO	000629-54-9	78
4	Tetradecanamide	227	C14H29NO	000638-58-4	78
5	Octadecanamide	283	C18H37NO	000124-26-5	59





Tentatively Identified Compound (LSC) summary

Data Path : U:\HPCHEM1\BNA_F\DATA\BF020518\
Data File : BF102745.D
Acq On : 5 Feb 2018 18:33
Operator : SJ/JU
Sample : J1456-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SA-ST-LATERAL-LINE-2-SW@4

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...	2.18	9.3	ng	625673	1	6.88	1348780	20.0
2-Pentanone, 4-hy...	5.12	3.0	ng	205889	1	6.88	1348780	20.0
unknown6.65	6.65	74.8	ng	5043800	1	6.88	1348780	20.0
Octadecane	9.85	2.4	ng	221113	3	9.92	1822210	20.0
Tetradecane	10.35	2.7	ng	246150	3	9.92	1822210	20.0
Hexadecane	10.82	3.5	ng	266121	4	11.40	1536430	20.0
n-Hexadecanoic acid	11.93	8.3	ng	639705	4	11.40	1536430	20.0
Octadecanoic acid	12.71	3.4	ng	264168	4	11.40	1536430	20.0
1-Heneicosanol	13.87	6.8	ng	368685	5	14.04	1086530	20.0
13-Docosenamide, ...	14.80	11.6	ng	615217	6	15.52	1063500	20.0