LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102866.D
Acq On : 8 Feb 2018 19:49
Operator : SJ/JU
Sample : J1470-17
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-13

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	2.163	8	13	20	rVB	448796	578207	12.43%	1.498%
2	5.116	512	515	524	rVB	131025	171438	3.68%	0.444%
3	5.504	576	581	585	rBV	4311703	4652823	100.00%	12.058%
4	6.516	747	753	764	rBV	4193541	4578668	98.41%	11.866%
5	6.657	772	777	780	rBV	4693906	4425065	95.10%	11.468%
6	6.886	812	816	819	rBV	1447827	1191517	25.61%	3.088%
7	7.039	838	842	846	rBV	3209248	3163371	67.99%	8.198%
8	7.445	906	911	915	rBV	2782296	2988456	64.23%	7.745%
9	7.522	921	924	934	rVV2	41443	52741	1.13%	0.137%
10	8.169	1030	1034	1037	rBV	1741189	1462296	31.43%	3.790%
11	9.239	1212	1216	1220	rBV	3518159	3501115	75.25%	9.074%
12	9.316	1226	1229	1232	rVB	117470	98340	2.11%	0.255%
13	9.574	1267	1273	1279	rBV3	47654	65905	1.42%	0.171%
14	9.633	1279	1283	1286	rBV	485183	420300	9.03%	1.089%
15	9.845	1312	1319	1322	rBV	272557	237003	5.09%	0.614%
16	9.922	1328	1332	1336	rBV	1451986	1369553	29.43%	3.549%
17	10.074	1354	1358	1361	rBV3	45144	53486	1.15%	0.139%
18	10.169	1371	1374	1378	rBV2	51150	53797	1.16%	0.139%
19	10.321	1397	1400	1402	rBV	49512	49197	1.06%	0.127%
20	10.345	1402	1404	1407	rVB	278457	198648	4.27%	0.515%
21	10.569	1437	1442	1444	rBV	67116	83900	1.80%	0.217%
22	10.716	1463	1467	1470	rBV	1915335	1894398	40.72%	4.910%
23	10.816	1481	1484	1494	rVB	257179	311409	6.69%	0.807%
24	11.268	1558	1561	1563	rBV	123244	103601	2.23%	0.268%
25	11.298	1563	1566	1572	rVB2	48681	57700	1.24%	0.150%
26	11.410	1582	1585	1589	rBV	1146621	1064286	22.87%	2.758%
27	11.692	1631	1633	1636	rBV	60752	48943	1.05%	0.127%
28	11.927	1670	1673	1682	rBV3	90652	112081	2.41%	0.290%
29	12.810	1820	1823	1826	rVB	70698	54976	1.18%	0.142%
30	12.998	1850	1855	1858	rBV	2516895	2318606	49.83%	6.009%
31	13.468	1932	1935	1941	rBV2	145351	163043	3.50%	0.423%
32	13.880	2002	2005	2017	rBV	740343	708469	15.23%	1.836%
33	14.051	2030	2034	2038	rBV	1000914	960411	20.64%	2.489%
34	14.515	2109	2113	2119	rBV2	115865	165229	3.55%	0.428%

LSC Area Percent Report

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Acq On : 8 Feb 2018 19:49
Operator : SJ/JU
Sample : J1470-17
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-13

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	15.162	2220	2223	2227	rBV	164124	197955	4.25%	0.513%
36	15.539	2283	2287	2295	rVB	584875	817551	17.57%	2.119%
37	15.998	2362	2365	2370	rVB	155767	211546	4.55%	0.548%

Sum of corrected areas: 38586030

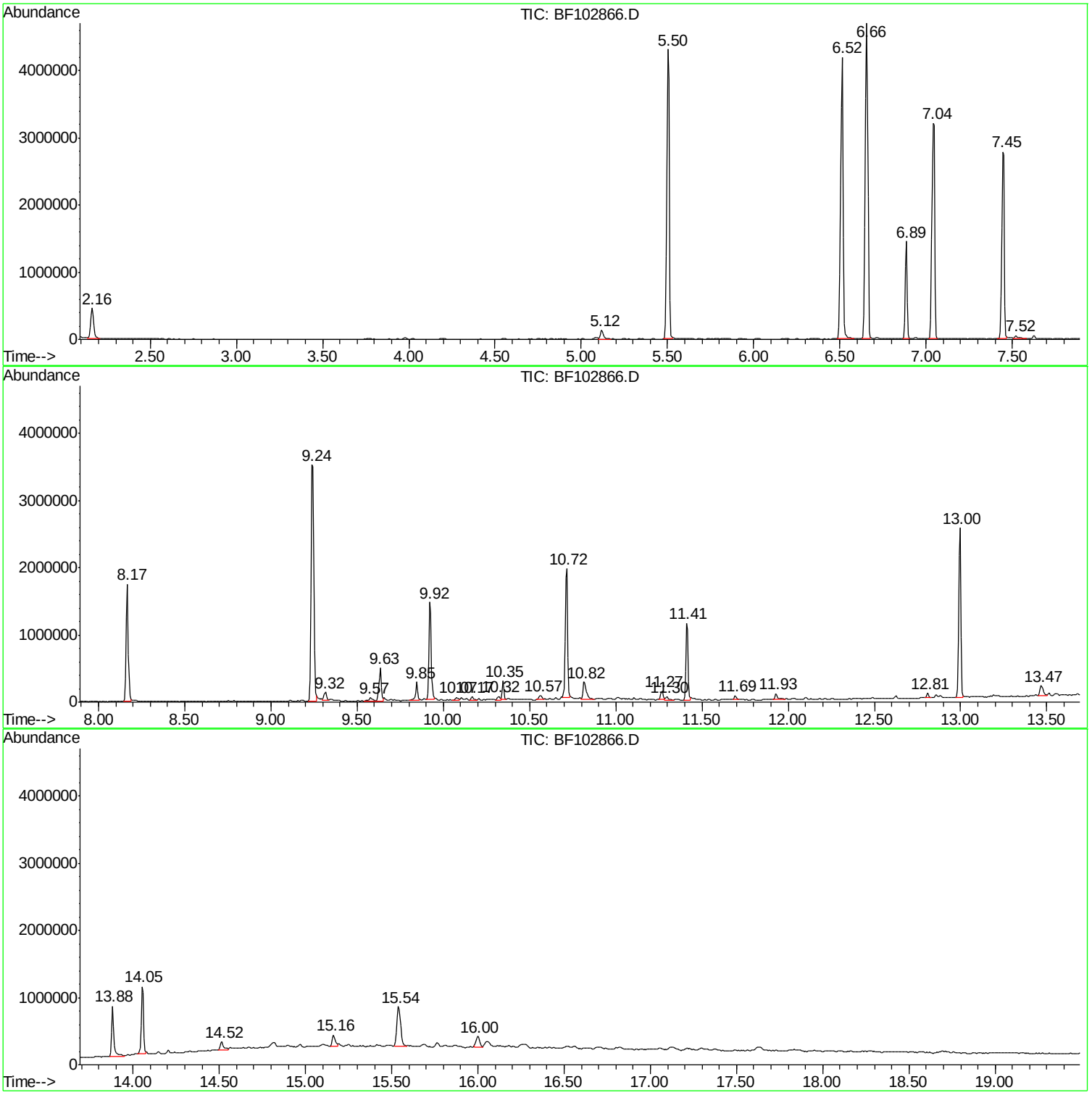
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102866.D
Acq On : 8 Feb 2018 19:49
Operator : SJ/JU
Sample : J1470-17
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-13

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 : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102866.D
Acq On : 8 Feb 2018 19:49
Operator : SJ/JU
Sample : J1470-17
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-13

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

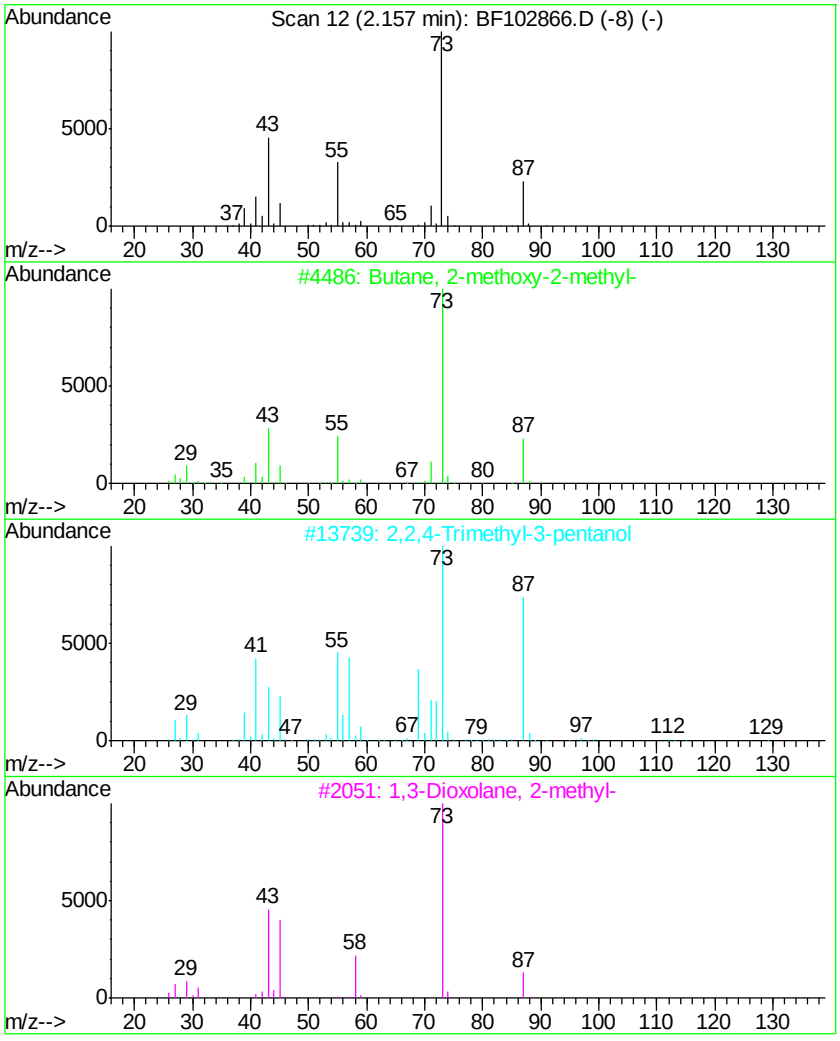
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

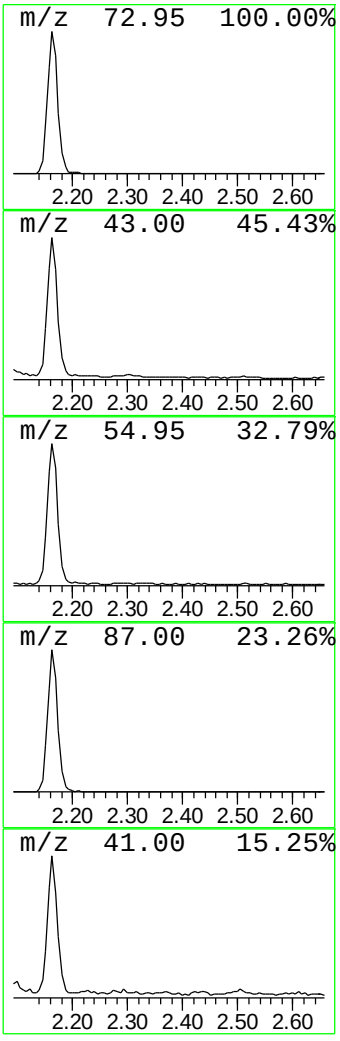
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	9.71 ng	578207	1,4-Dichlorobenzene-d4	6.89

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Operator : SJ/JU
Sample : J1470-17
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-13

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

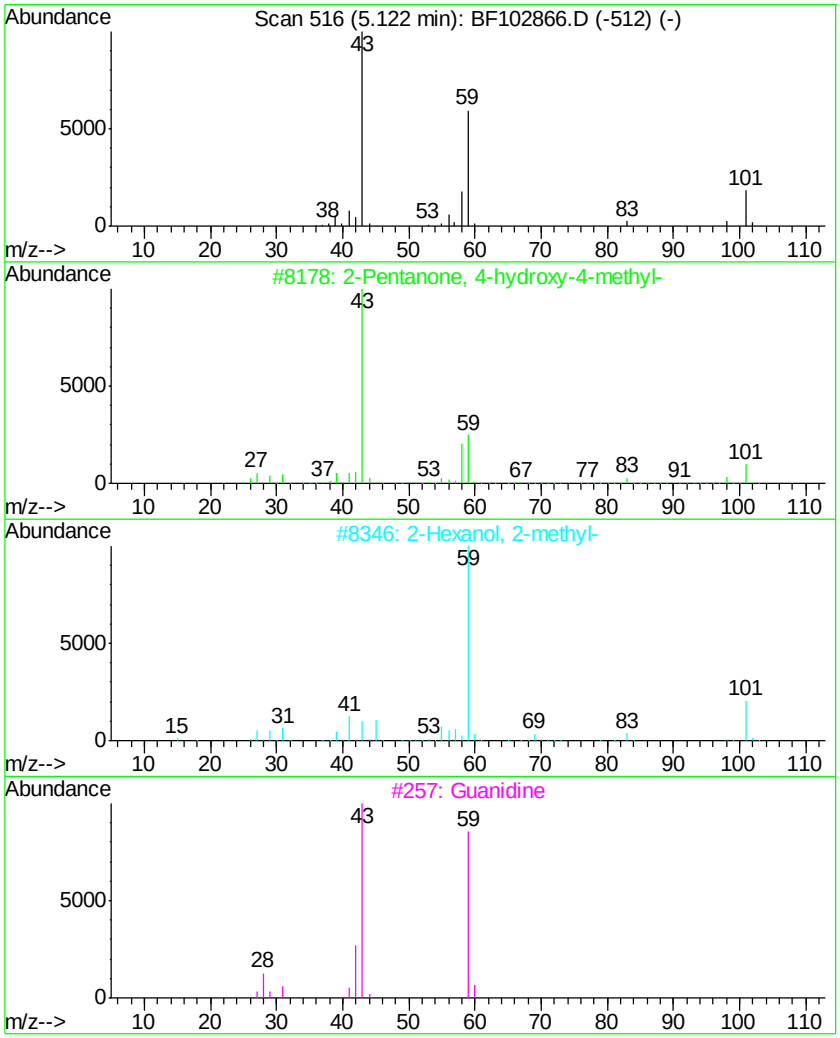
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

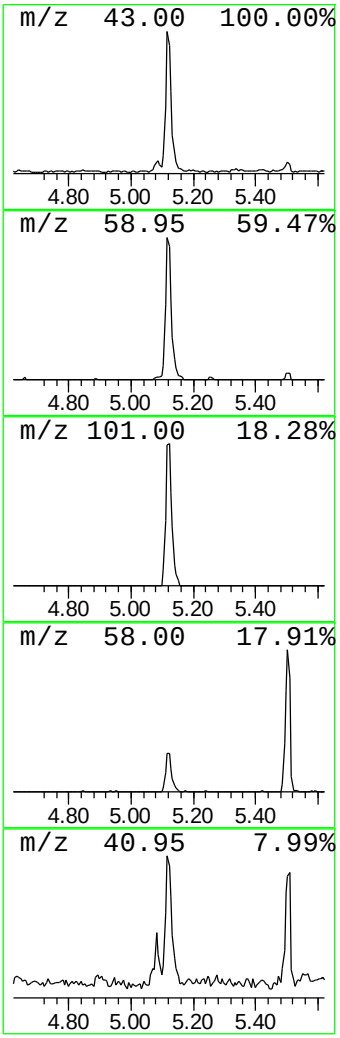
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	2.88 ng	171438	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3	Guanidine	59	CH5N3	000113-00-8	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





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Data File : BF102866.D
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Operator : SJ/JU
Sample : J1470-17
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-13

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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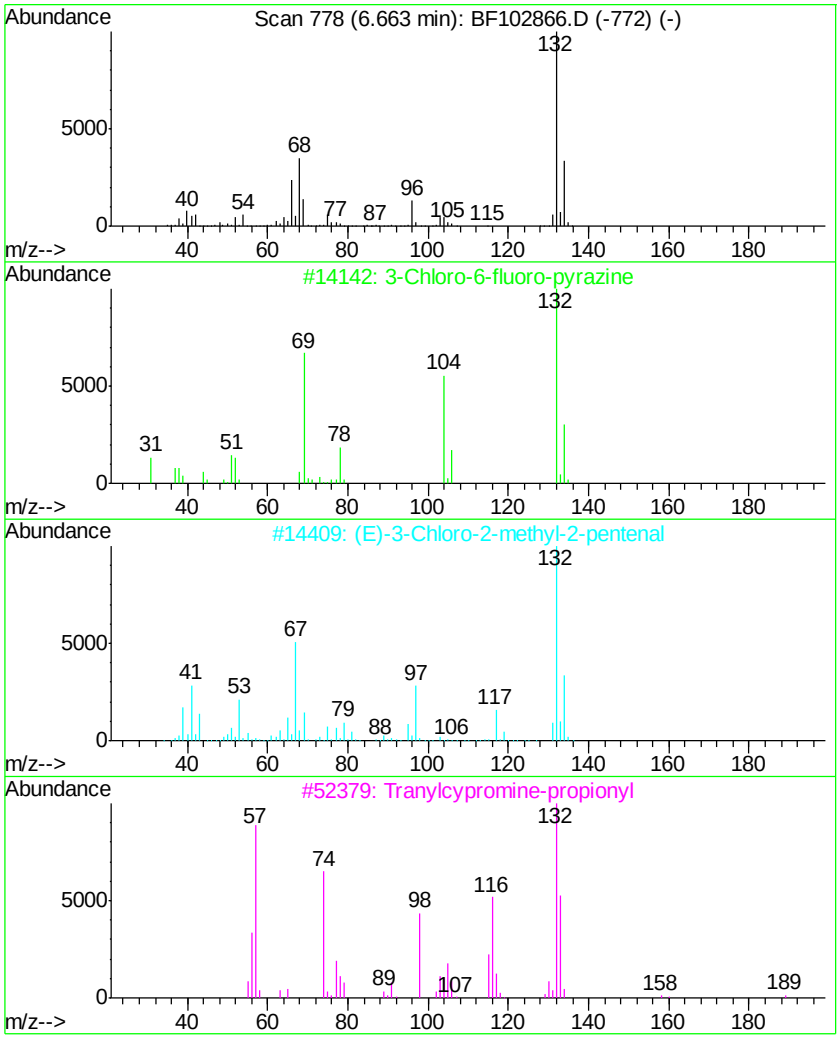
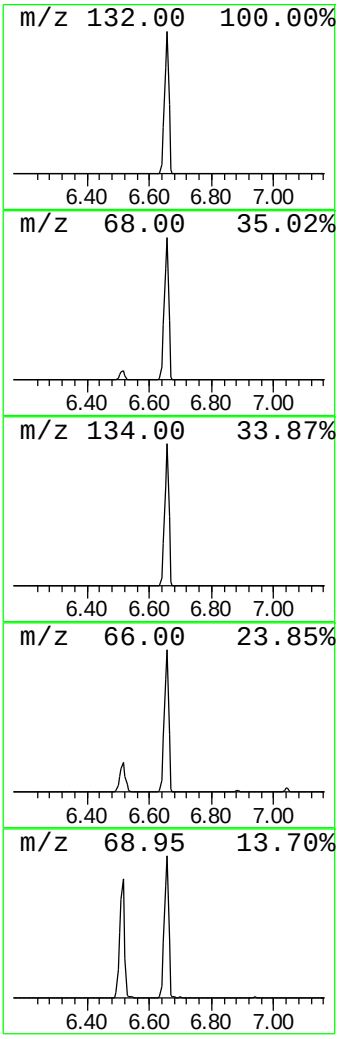
Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	74.28 ng	4425070	1,4-Dichlorobenzene-d4	6.89

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	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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Data File : BF102866.D
Acq On : 8 Feb 2018 19:49
Operator : SJ/JU
Sample : J1470-17
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-13

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

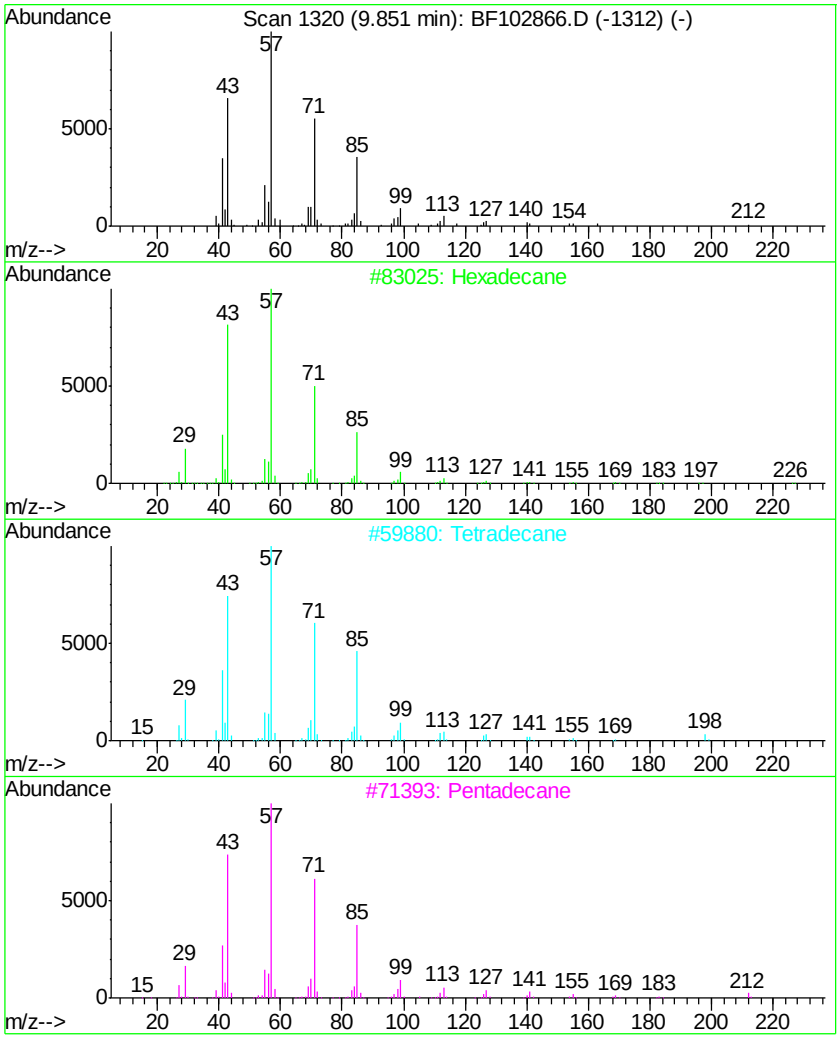
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

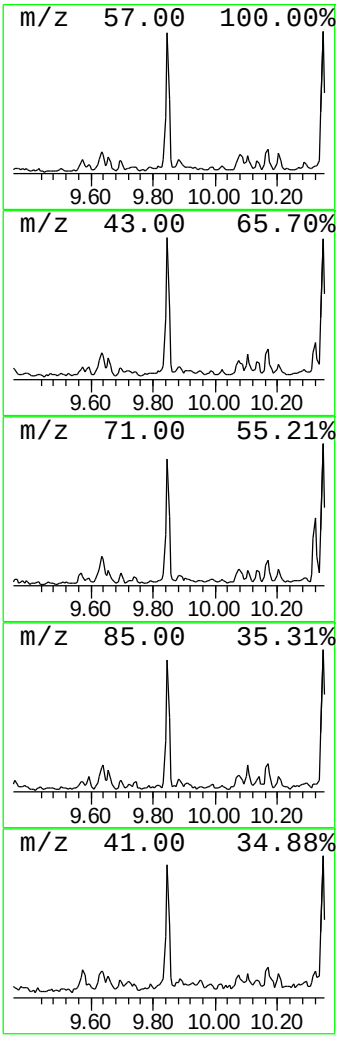
****

Peak Number 5 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.85	3.46 ng	237003	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Tetradecane	198	C14H30	000629-59-4	90
3	Pentadecane	212	C15H32	000629-62-9	86
4	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	80
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78





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Sample : J1470-17
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-13

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

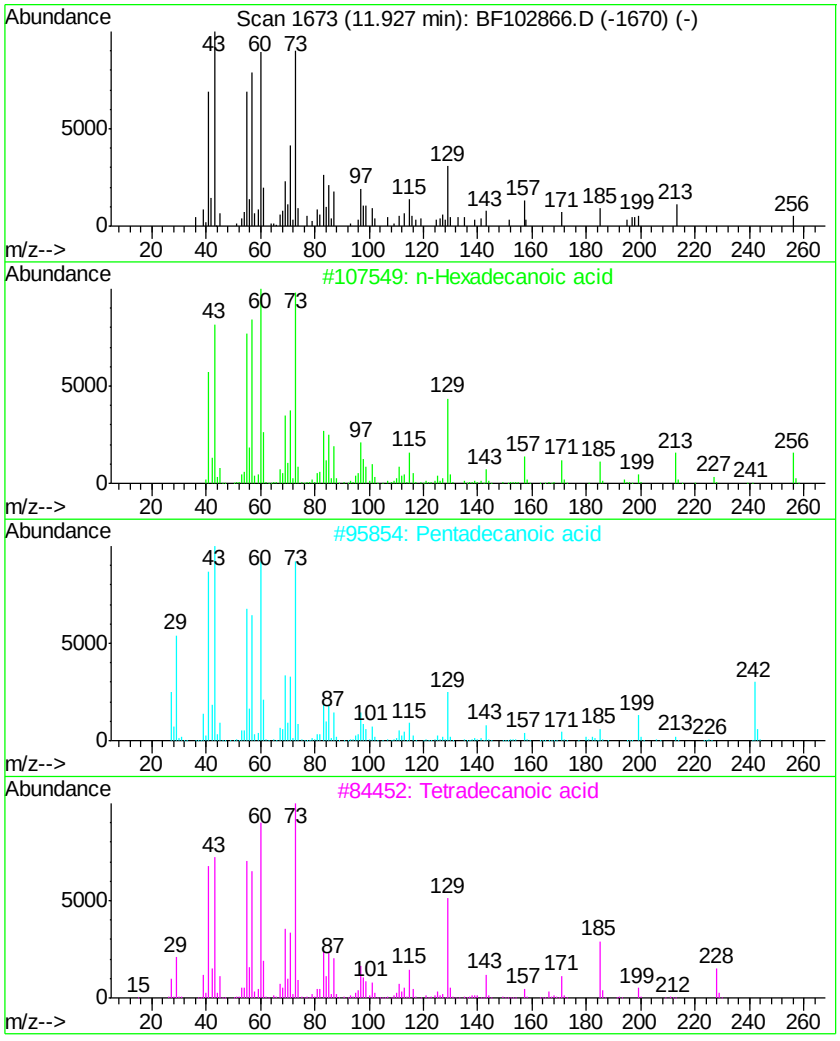
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

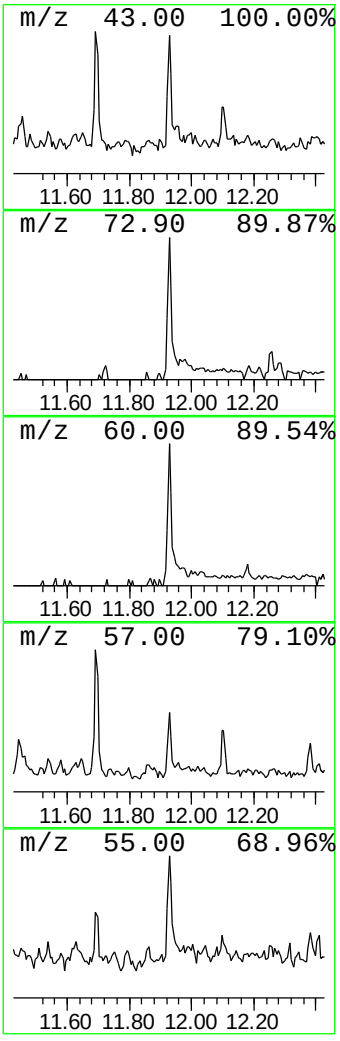
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	2.11 ng	112081	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	72





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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

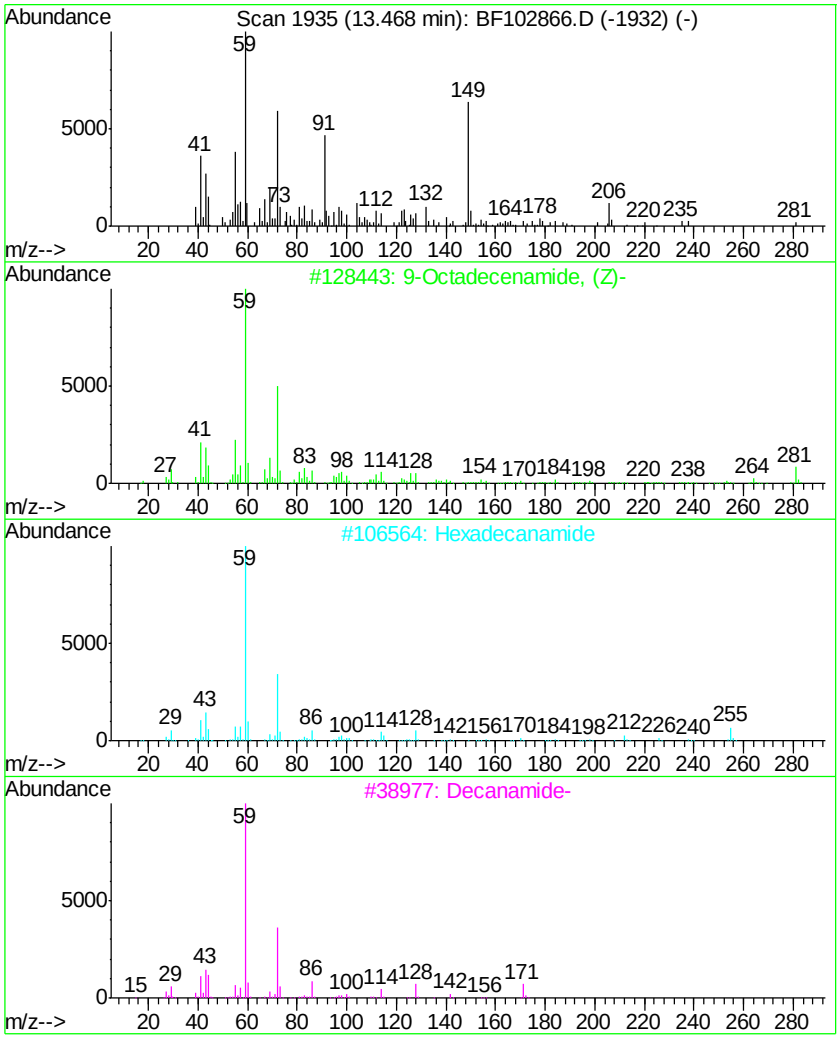
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

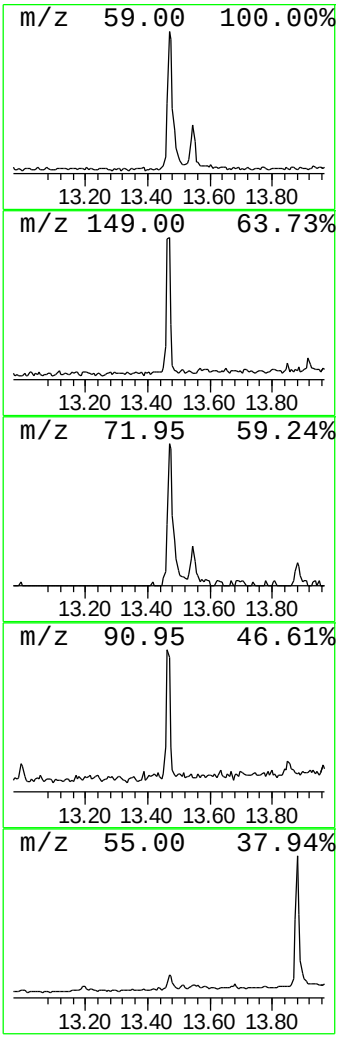
****

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	3.40 ng	163043	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	58
2	Hexadecanamide	255	C16H33NO	000629-54-9	43
3	Decanamide-	171	C10H21NO	002319-29-1	43
4	Dodecanamide	199	C12H25NO	001120-16-7	43
5	2-Heptanol, 2,6-dimethyl-	144	C9H20O	013254-34-7	27





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BNA_F
ClientSampleId :
3N-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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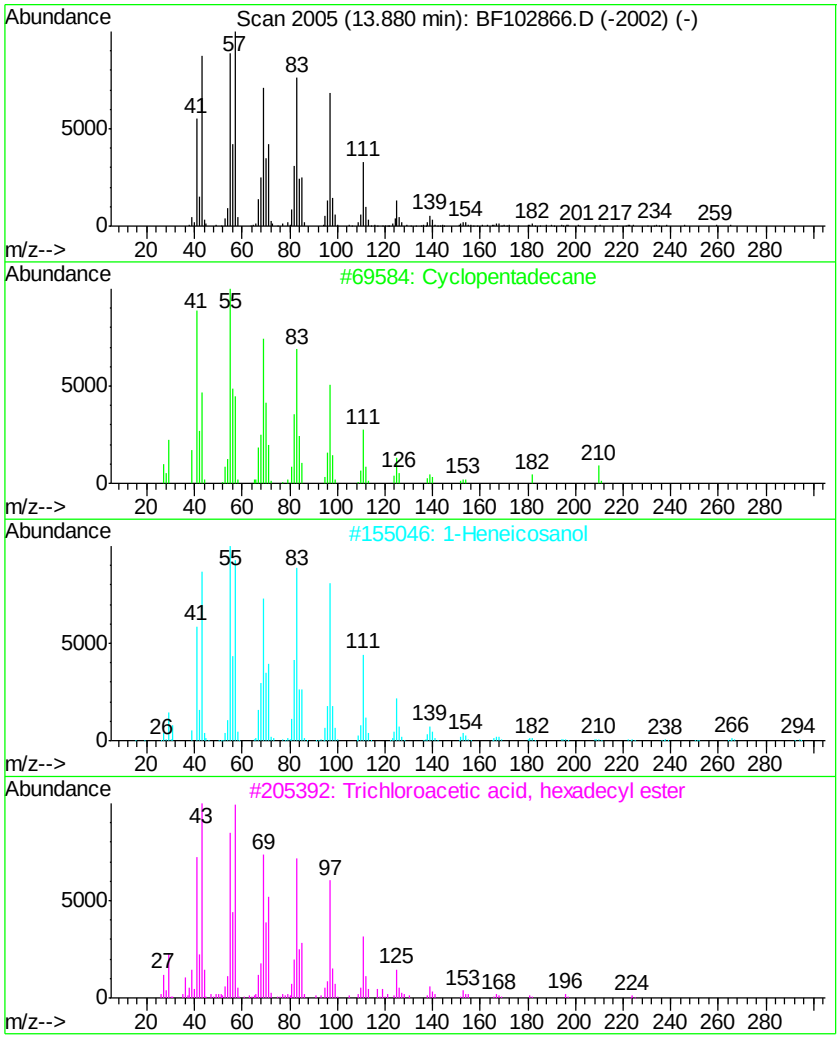
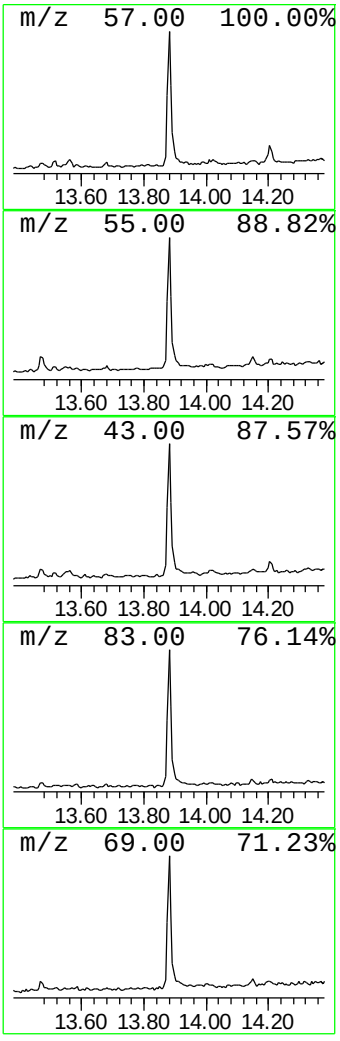
Peak Number 10 Cyclopentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	14.75 ng	708469	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	96
2	1-Heneicosanol	312	C21H44O	015594-90-8	94
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4	1-Docosene	308	C22H44	001599-67-3	94
5	1-Octadecanol	270	C18H38O	000112-92-5	91





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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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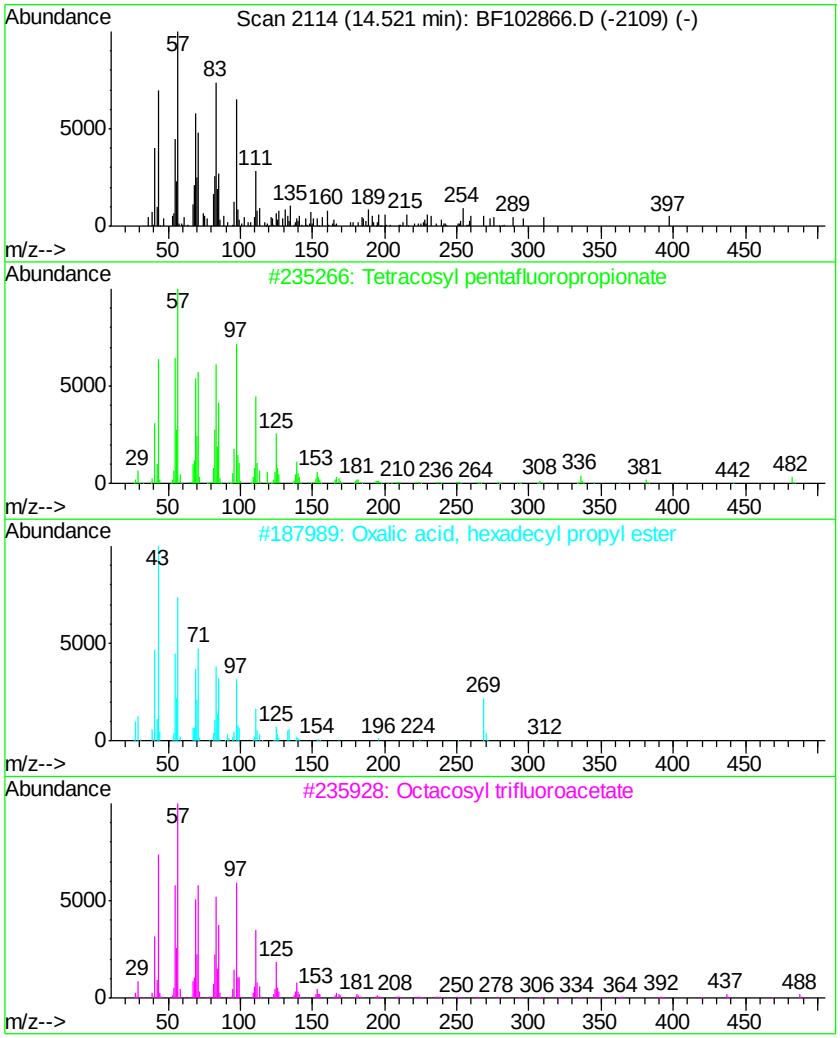
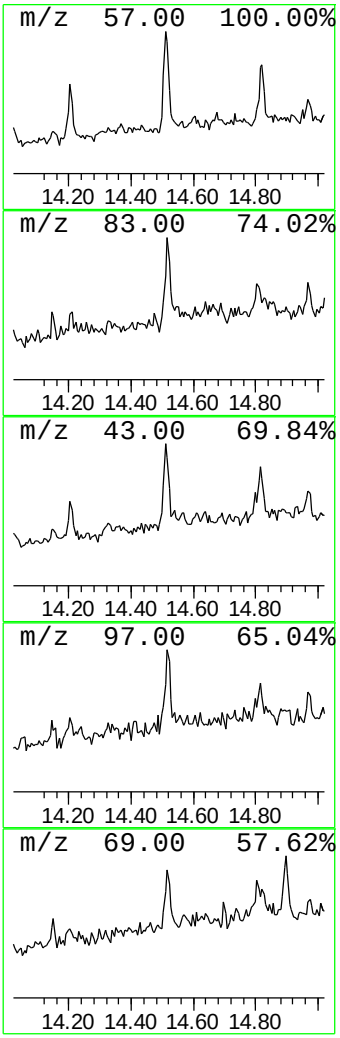
Peak Number 11 Tetracosyl pentafluoropropi... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	3.44 ng	165229	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosyl pentafluoropropionate	500	C27H49F5O2	1000351-81-3	90
2	Oxalic acid, hexadecyl propyl ester	356	C21H40O4	1000309-26-9	90
3	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	80
4	Decane	142	C10H22	000124-18-5	70
5	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	64





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Misc :
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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

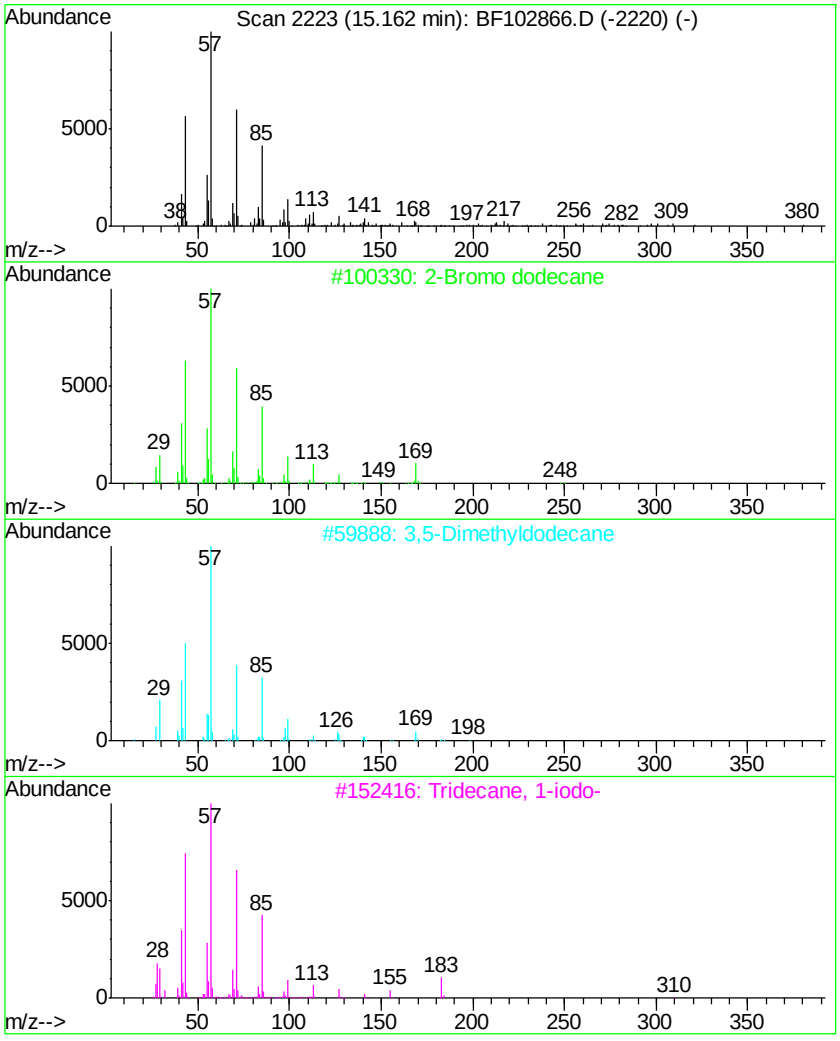
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

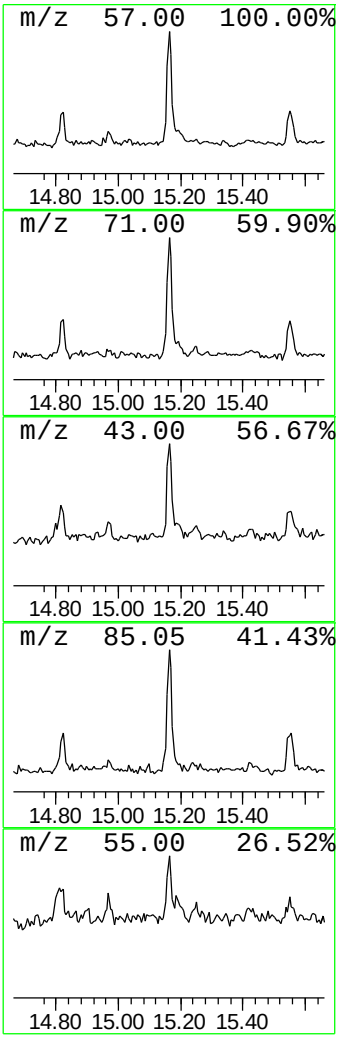
****

Peak Number 12 2-Bromo dodecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	4.84 ng	197955	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	91
2	3,5-Dimethyldodecane	198	C14H30	107770-99-0	83
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
4	1-Iodoundecane	282	C11H23I	004282-44-4	80
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	72





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102866.D
Acq On : 8 Feb 2018 19:49
Operator : SJ/JU
Sample : J1470-17
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-13

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

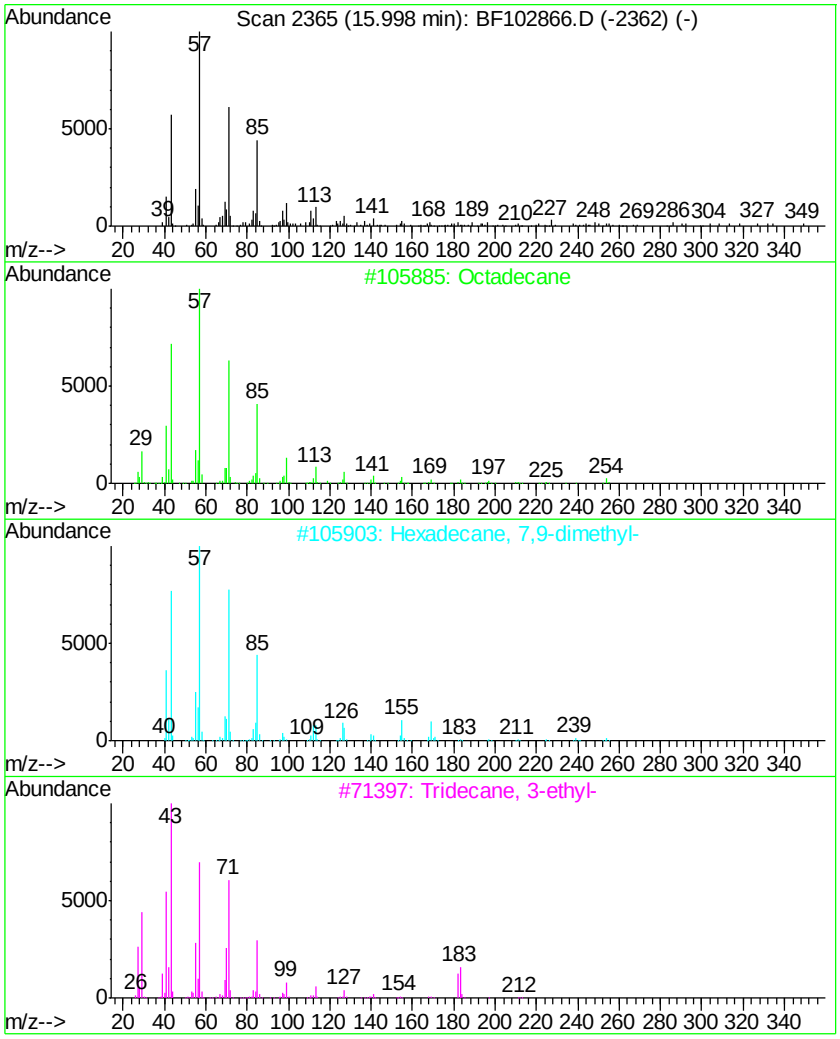
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

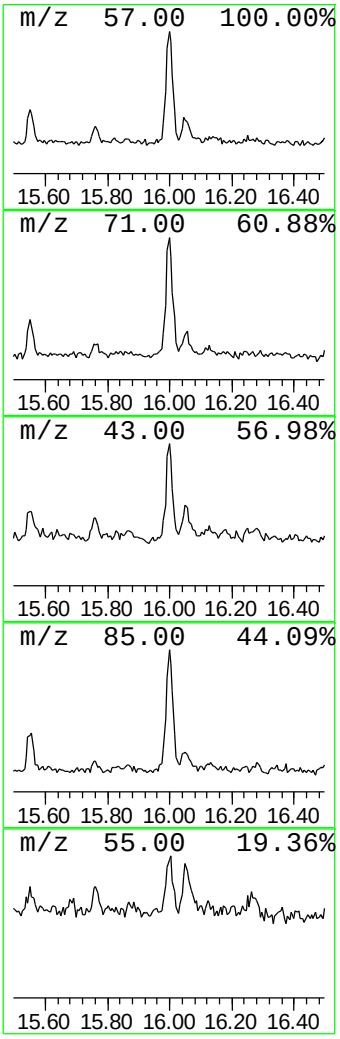
****

Peak Number 13 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.00	5.18 ng	211546	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	93
2	Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	90
3	Tridecane, 3-ethyl-	212	C15H32	013286-73-2	90
4	Heptacosane	380	C27H56	000593-49-7	87
5	Tetracosane	338	C24H50	000646-31-1	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102866.D
Acq On : 8 Feb 2018 19:49
Operator : SJ/JU
Sample : J1470-17
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-13

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...	2.16	9.7	ng	578207	1	6.89	1191520	20.0
2-Pentanone, 4-hy...	5.12	2.9	ng	171438	1	6.89	1191520	20.0
unknown6.66	6.66	74.3	ng	4425070	1	6.89	1191520	20.0
Hexadecane	9.85	3.5	ng	237003	3	9.92	1369550	20.0
n-Hexadecanoic acid	11.93	2.1	ng	112081	4	11.41	1064290	20.0
9-Octadecenamide,...	13.47	3.4	ng	163043	5	14.05	960411	20.0
Cyclopentadecane	13.88	14.8	ng	708469	5	14.05	960411	20.0
Tetracosyl pentaf...	14.52	3.4	ng	165229	5	14.05	960411	20.0
2-Bromo dodecane	15.16	4.8	ng	197955	6	15.54	817551	20.0
Octadecane	16.00	5.2	ng	211546	6	15.54	817551	20.0