LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102766.D
Acq On : 6 Feb 2018 4:51
Operator : SJ/JU
Sample : J1454-06
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-SAN-6-EW(4-8)

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	2.193	12	18	29	rVB	567495	765823	14.96%	1.584%
2	5.122	513	516	522	rVB	149040	194692	3.80%	0.403%
3	5.504	575	581	584	rBV	4704718	5118925	100.00%	10.590%
4	6.510	743	752	755	rBV	4316085	5103441	99.70%	10.558%
5	6.563	758	761	767	rVB	65873	63892	1.25%	0.132%
6	6.651	771	776	779	rVV	4998673	4960364	96.90%	10.262%
7	6.704	782	785	790	rVB	262883	213413	4.17%	0.442%
8	6.881	811	815	819	rVB	1794906	1425819	27.85%	2.950%
9	6.933	821	824	827	rBV	61190	54478	1.06%	0.113%
10	7.039	837	842	844	rBV	3984118	3603797	70.40%	7.456%
11	7.063	844	846	850	rVB	91879	73571	1.44%	0.152%
12	7.128	854	857	859	rBV	80120	65840	1.29%	0.136%
13	7.151	859	861	864	rVB	85158	61178	1.20%	0.127%
14	7.198	864	869	871	rBV	172513	154084	3.01%	0.319%
15	7.416	902	906	907	rBV	244252	257026	5.02%	0.532%
16	7.445	907	911	914	rVB	3241339	3223528	62.97%	6.669%
17	7.645	943	945	947	rVV	145284	111727	2.18%	0.231%
18	7.675	947	950	953	rVB	146915	132702	2.59%	0.275%
19	7.763	960	965	967	rBV2	55407	56151	1.10%	0.116%
20	7.810	970	973	975	rVV	53753	55299	1.08%	0.114%
21	7.833	975	977	981	rVV3	117714	127711	2.49%	0.264%
22	7.898	985	988	991	rVV	232075	205296	4.01%	0.425%
23	7.928	991	993	995	rVB2	76837	58857	1.15%	0.122%
24	8.163	1027	1033	1036	rBV	2289695	2071155	40.46%	4.285%
25	8.204	1039	1040	1045	rVB2	63674	66959	1.31%	0.139%
26	8.545	1094	1098	1101	rBV2	56398	54996	1.07%	0.114%
27	8.875	1151	1154	1157	rVB	75820	59858	1.17%	0.124%
28	8.975	1167	1171	1175	rVB	66905	57609	1.13%	0.119%
29	9.239	1210	1216	1219	rBV	5002744	4583148	89.53%	9.482%
30	9.627	1279	1282	1285	rBV	419279	331383	6.47%	0.686%
31	9.845	1316	1319	1321	rVB	135964	121340	2.37%	0.251%
32	9.916	1327	1331	1335	rBV	1947825	1921595	37.54%	3.975%
33	10.345	1401	1404	1407	rVB	203869	162037	3.17%	0.335%
34	10.563	1436	1441	1444	rBV	54954	71604	1.40%	0.148%

LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102766.D
Acq On : 6 Feb 2018 4:51
Operator : SJ/JU
Sample : J1454-06
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-SAN-6-EW(4-8)

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	10.704	1459	1465	1469	rBV	2579764	2676162	52.28%	5.536%
36	10.816	1481	1484	1490	rBV	209111	186714	3.65%	0.386%
37	11.263	1557	1560	1563	rBV	92221	75584	1.48%	0.156%
38	11.404	1580	1584	1587	rBV	1900940	1624615	31.74%	3.361%
39	11.427	1587	1588	1591	rVB	144781	77567	1.52%	0.160%
40	11.927	1665	1673	1681	rBV	500084	588673	11.50%	1.218%
41	12.615	1787	1790	1794	rBV	163756	145437	2.84%	0.301%
42	12.710	1802	1806	1813	rBV	93489	112508	2.20%	0.233%
43	12.804	1819	1822	1824	rBV	122033	97709	1.91%	0.202%
44	12.845	1824	1829	1833	rVV	117827	138035	2.70%	0.286%
45	12.992	1849	1854	1857	rBV	3128879	3079709	60.16%	6.371%
46	13.462	1930	1934	1939	rVB	67612	66856	1.31%	0.138%
47	13.874	2001	2004	2013	rVB	988383	852885	16.66%	1.764%
48	14.039	2026	2032	2035	rBV	1158309	1209554	23.63%	2.502%
49	14.509	2108	2112	2117	rBV	124430	144380	2.82%	0.299%
50	14.798	2157	2161	2168	rBV2	92334	175458	3.43%	0.363%
51	15.080	2206	2209	2212	rBV	37079	51441	1.00%	0.106%
52	15.521	2278	2284	2293	rBV	820306	1087359	21.24%	2.250%
53	15.992	2360	2364	2367	rBV	39583	51930	1.01%	0.107%
54	16.039	2367	2372	2380	rVV	131091	200126	3.91%	0.414%
55	17.609	2633	2639	2645	rVB	46710	104909	2.05%	0.217%

Sum of corrected areas: 48336909

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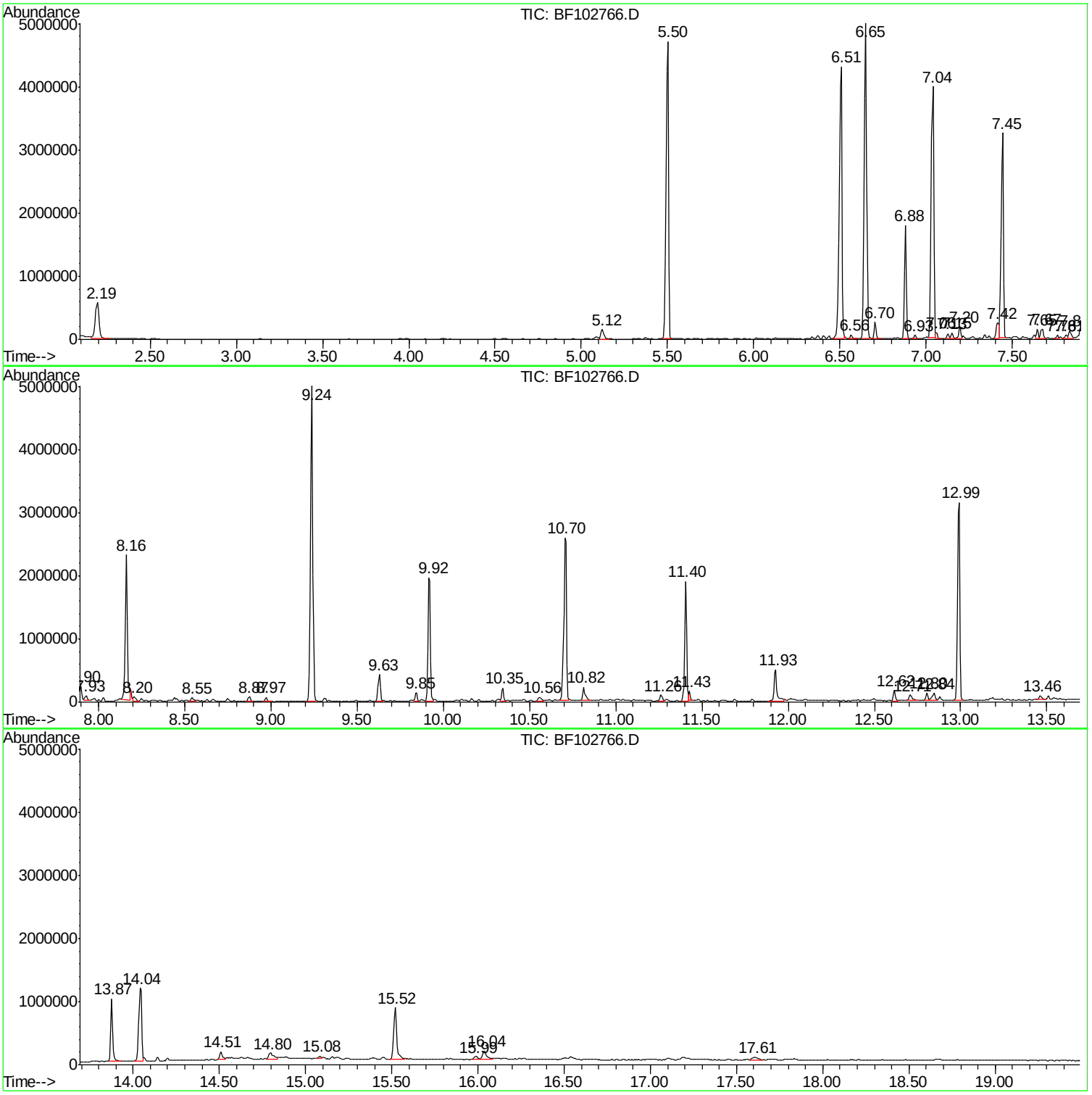
Data File : BF102766.D
Acq On : 6 Feb 2018 4:51
Operator : SJ/JU
Sample : J1454-06
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
8-SAN-6-EW(4-8)

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 : BF102766.D
Acq On : 6 Feb 2018 4:51
Operator : SJ/JU
Sample : J1454-06
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-SAN-6-EW(4-8)

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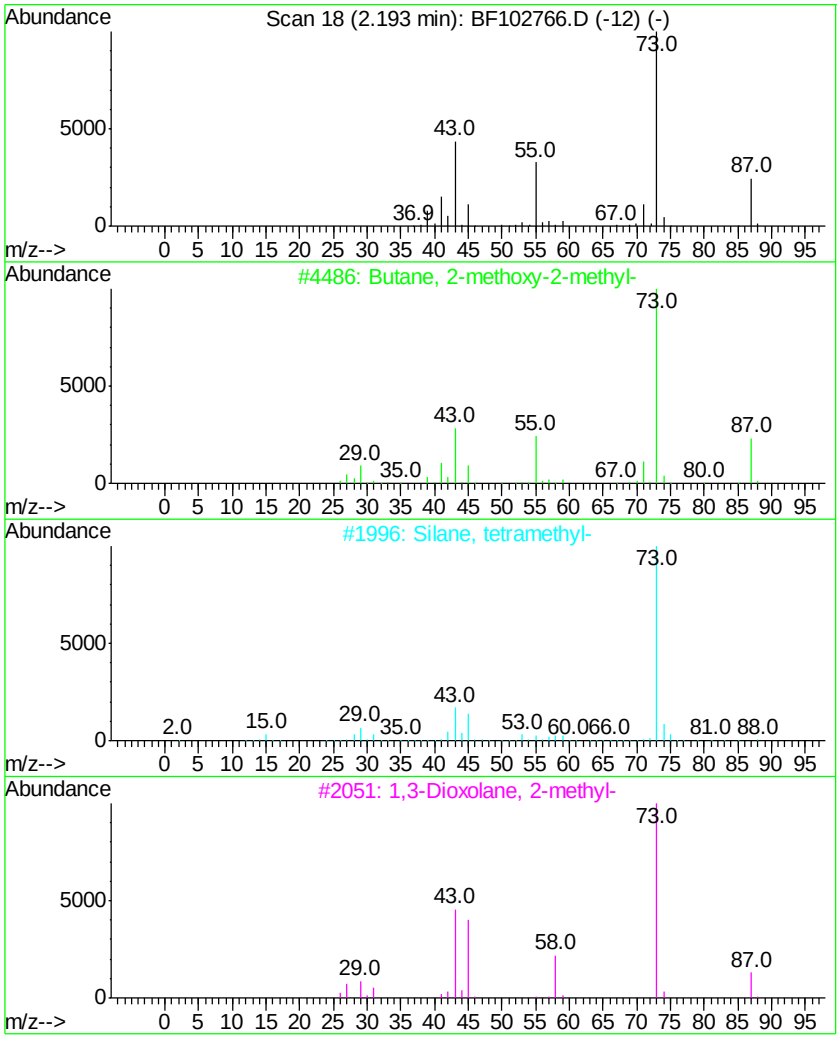
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

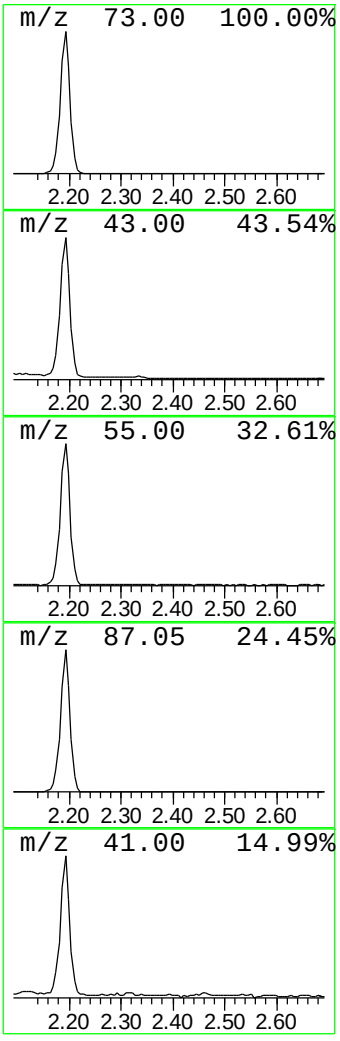
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.19	10.74 ng	765823	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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102766.D
Acq On : 6 Feb 2018 4:51
Operator : SJ/JU
Sample : J1454-06
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-SAN-6-EW(4-8)

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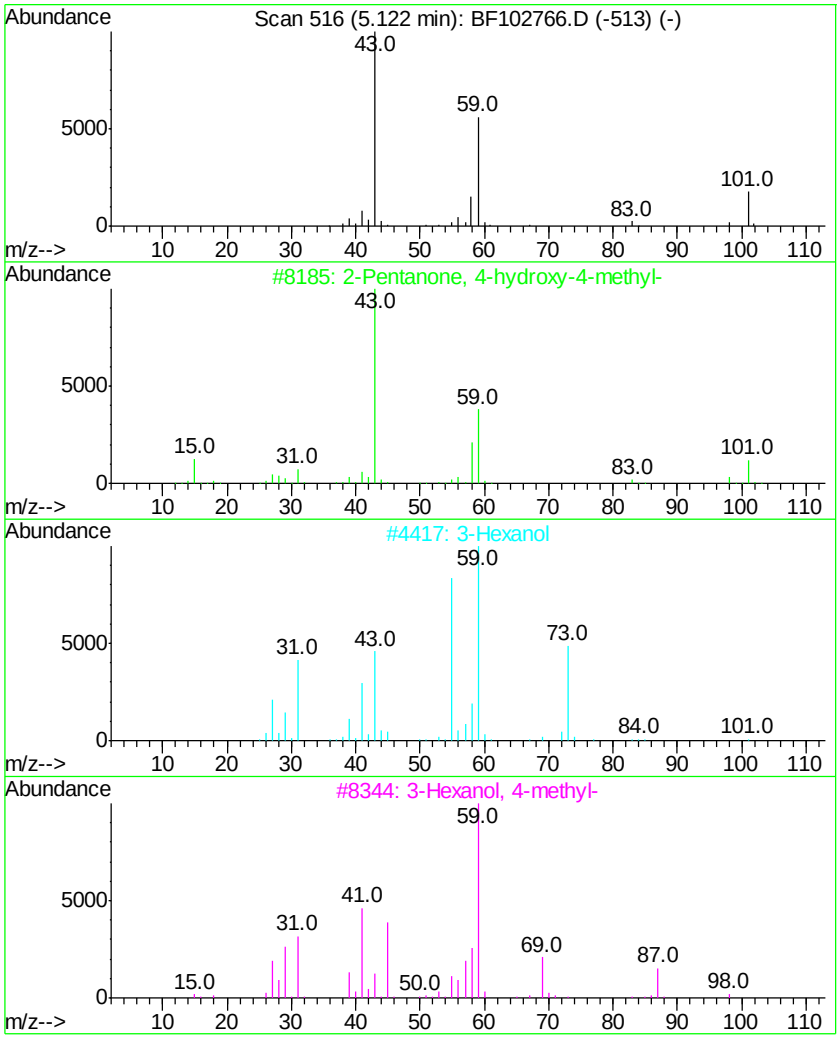
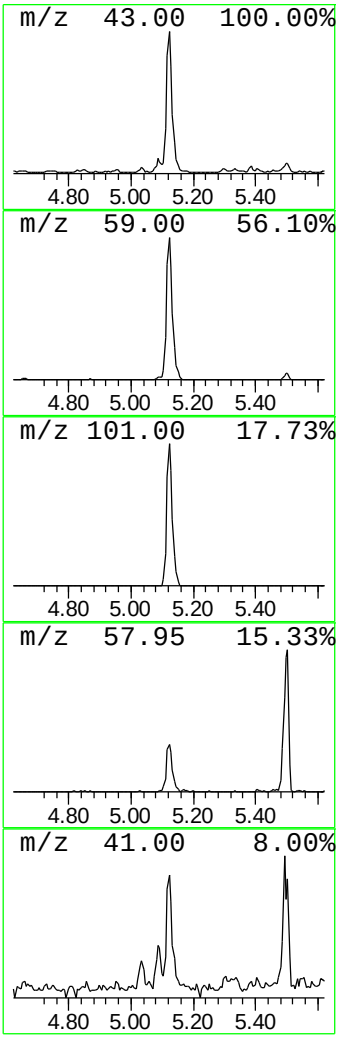
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	2.73 ng	194692	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	45
2	3-Hexanol	102	C6H14O	000623-37-0	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102766.D
Acq On : 6 Feb 2018 4:51
Operator : SJ/JU
Sample : J1454-06
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-SAN-6-EW(4-8)

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

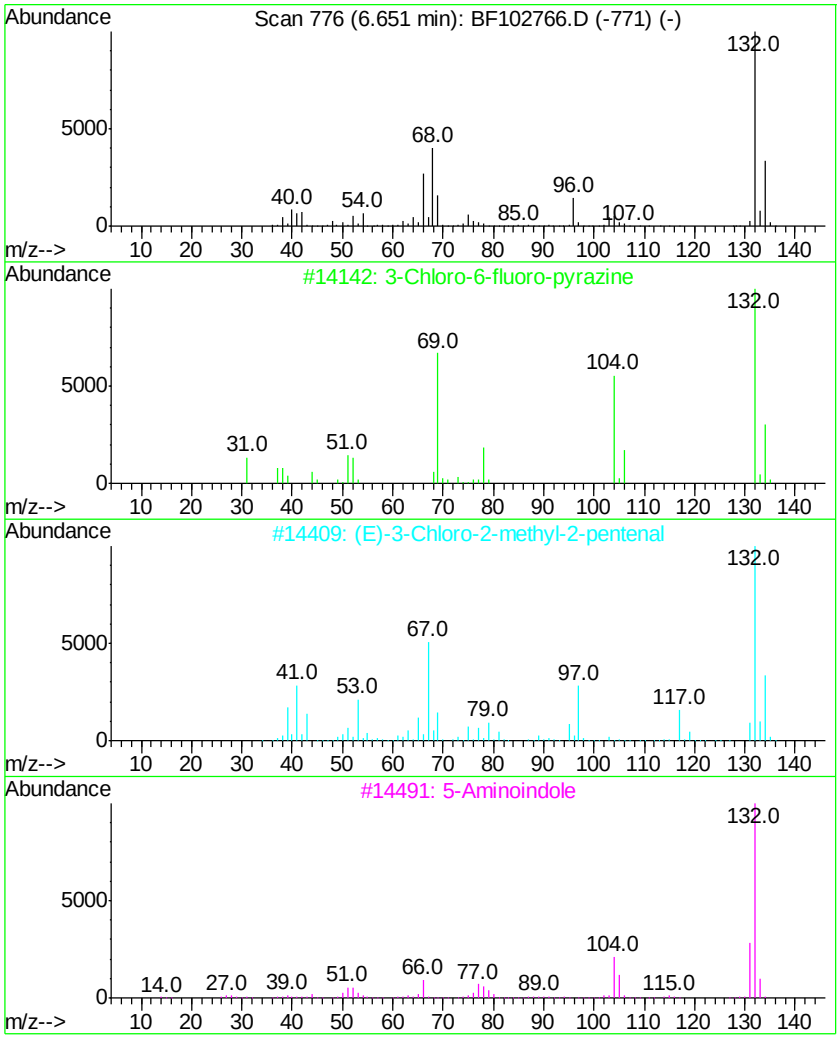
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

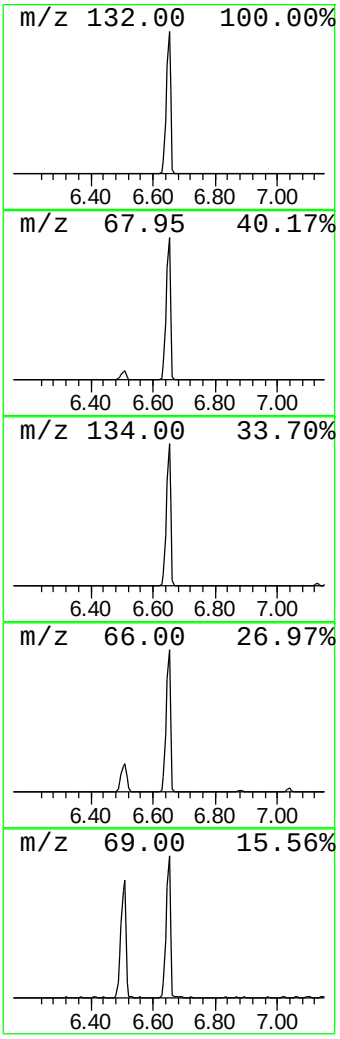
****

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	69.58 ng	4960360	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	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102766.D
Acq On : 6 Feb 2018 4:51
Operator : SJ/JU
Sample : J1454-06
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-SAN-6-EW(4-8)

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

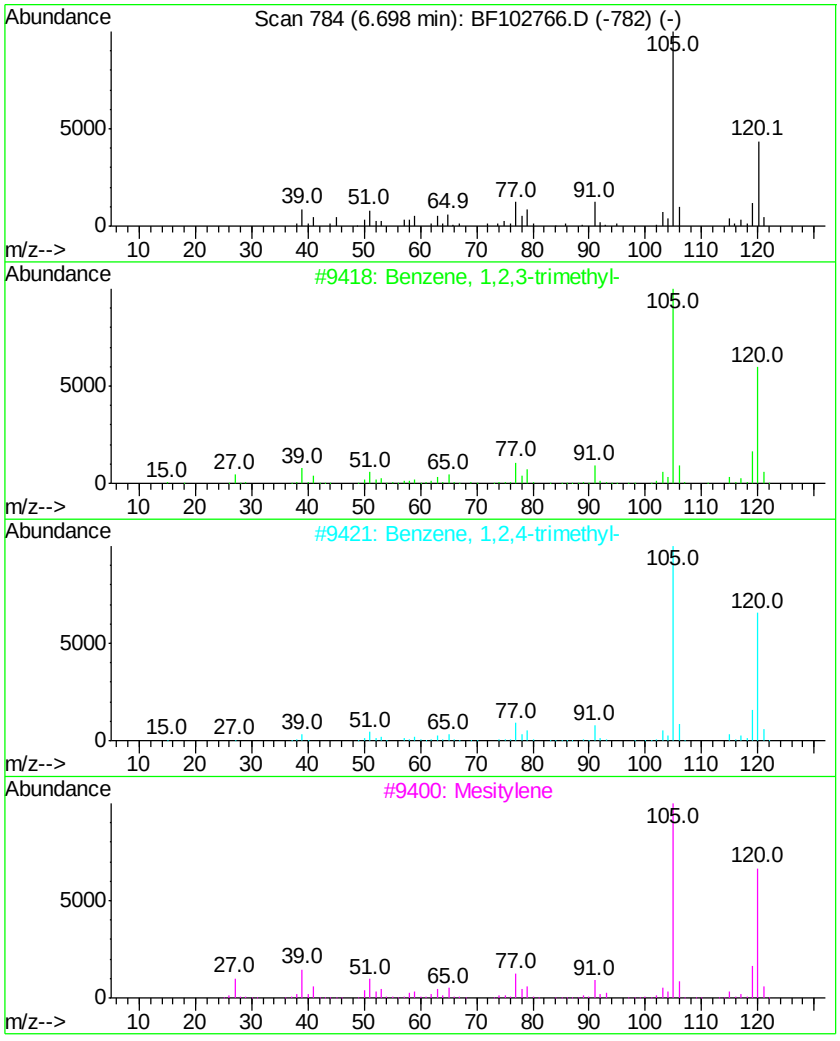
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

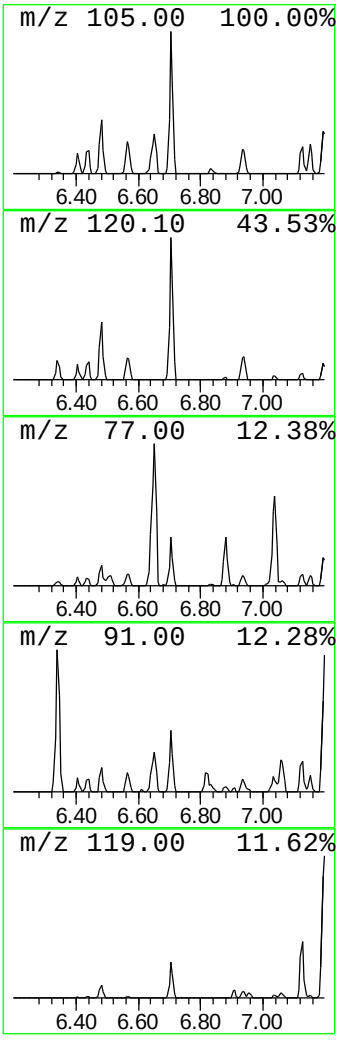
****

Peak Number 4 Benzene, 1,2,3-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	2.99 ng	213413	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	95
3	Mesitylene	120	C9H12	000108-67-8	94
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90





Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102766.D
Acq On : 6 Feb 2018 4:51
Operator : SJ/JU
Sample : J1454-06
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-SAN-6-EW(4-8)

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

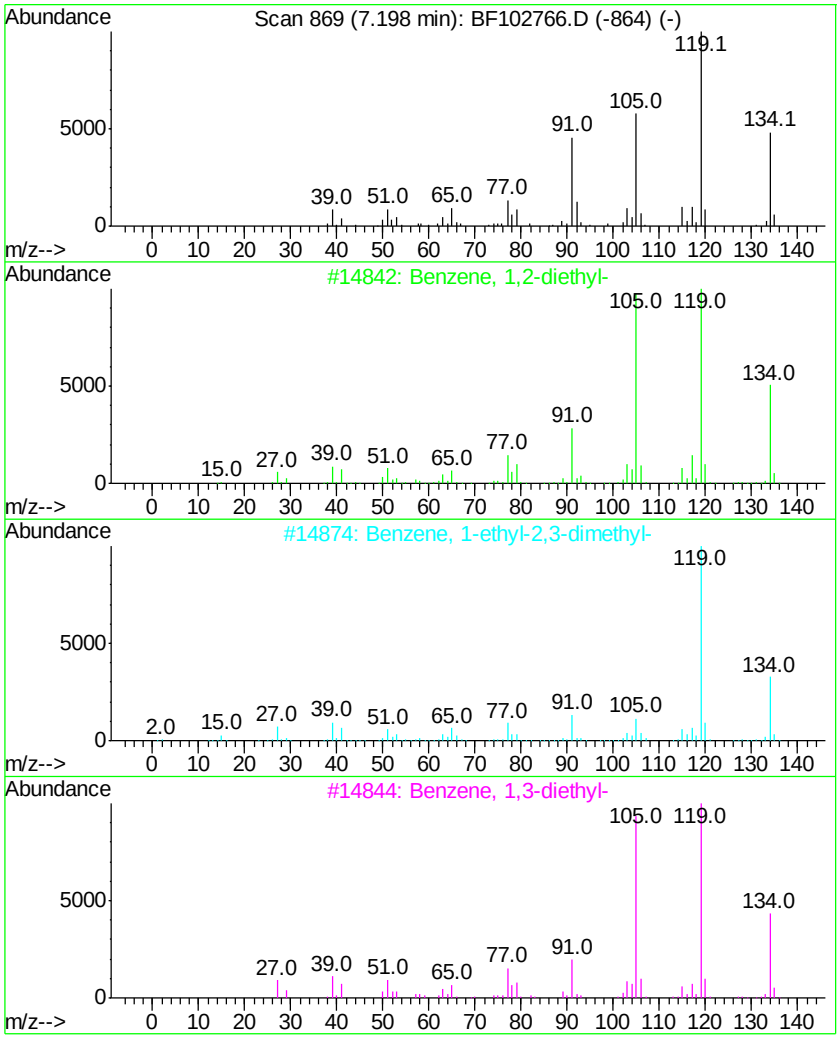
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

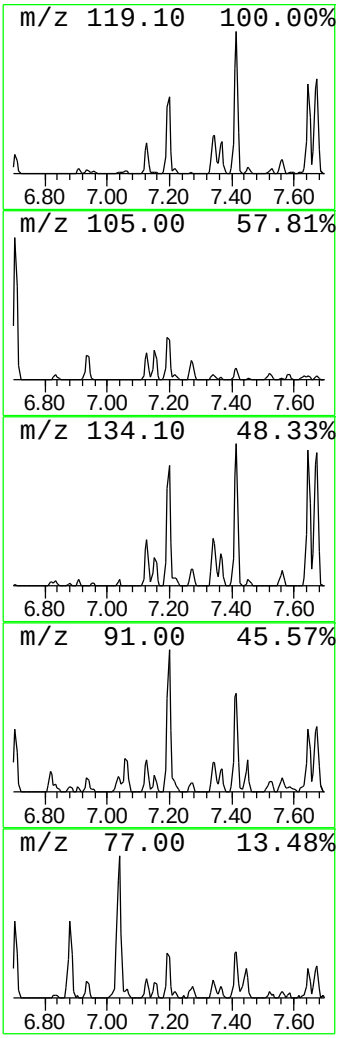
****

Peak Number 6 Benzene, 1,2-diethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	2.16 ng	154084	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	95
2	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	94
3	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	93
4	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	91
5	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91





Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102766.D
Acq On : 6 Feb 2018 4:51
Operator : SJ/JU
Sample : J1454-06
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-SAN-6-EW(4-8)

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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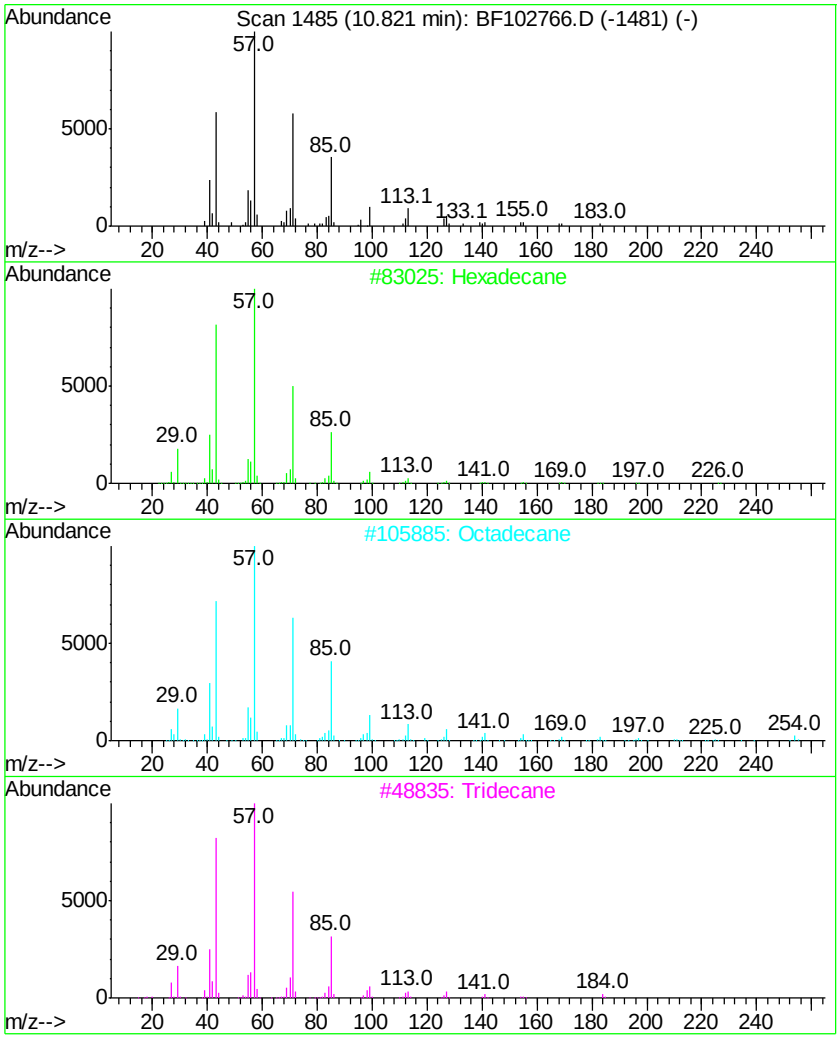
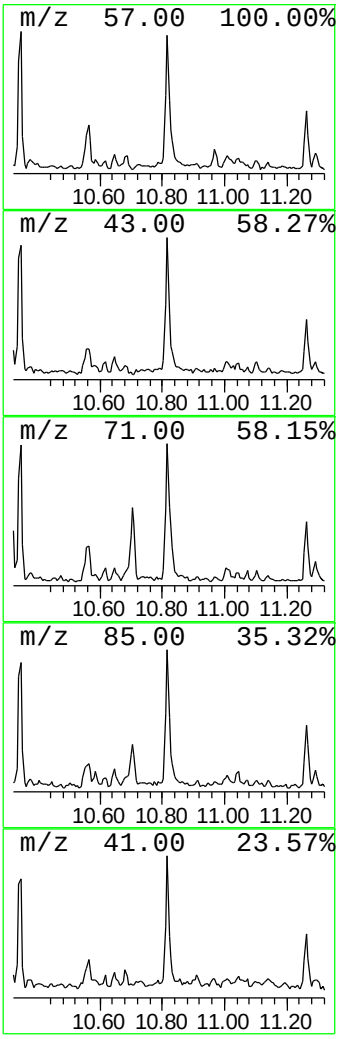
Peak Number 7 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	2.30 ng	186714	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Octadecane	254	C18H38	000593-45-3	90
3	Tridecane	184	C13H28	000629-50-5	86
4	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86
5	Tetratetracontane	619	C44H90	007098-22-8	83





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Data File : BF102766.D
Acq On : 6 Feb 2018 4:51
Operator : SJ/JU
Sample : J1454-06
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-SAN-6-EW(4-8)

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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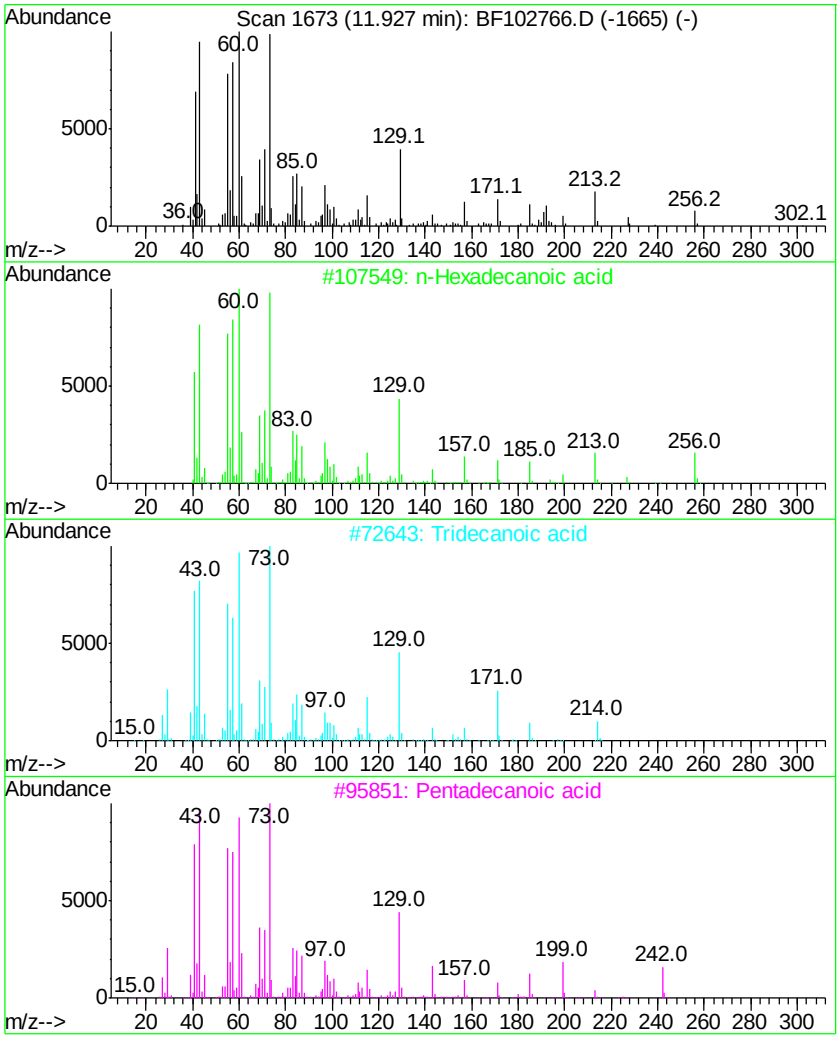
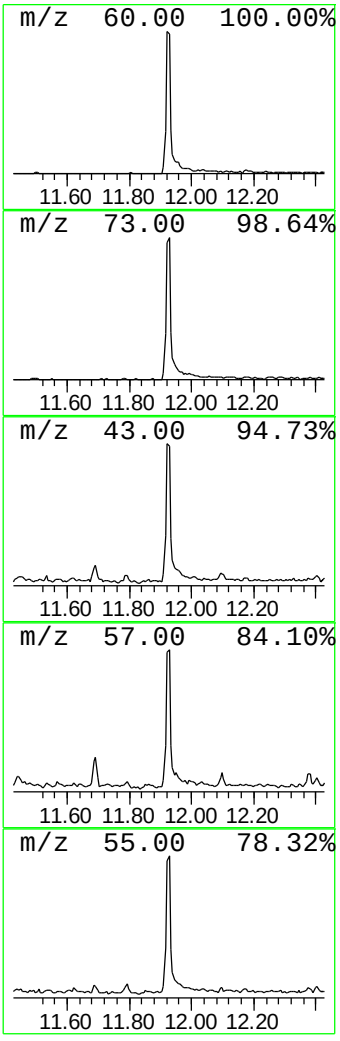
Peak Number 8 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	7.25 ng	588673	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	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102766.D
Acq On : 6 Feb 2018 4:51
Operator : SJ/JU
Sample : J1454-06
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-SAN-6-EW(4-8)

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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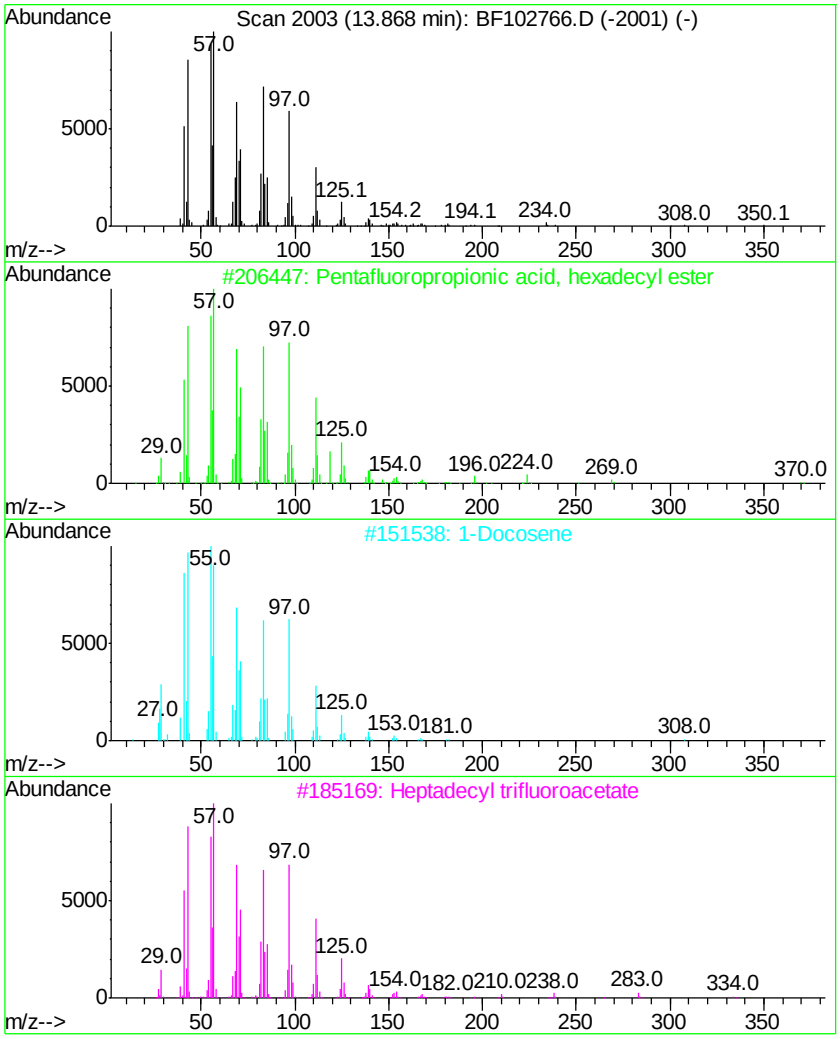
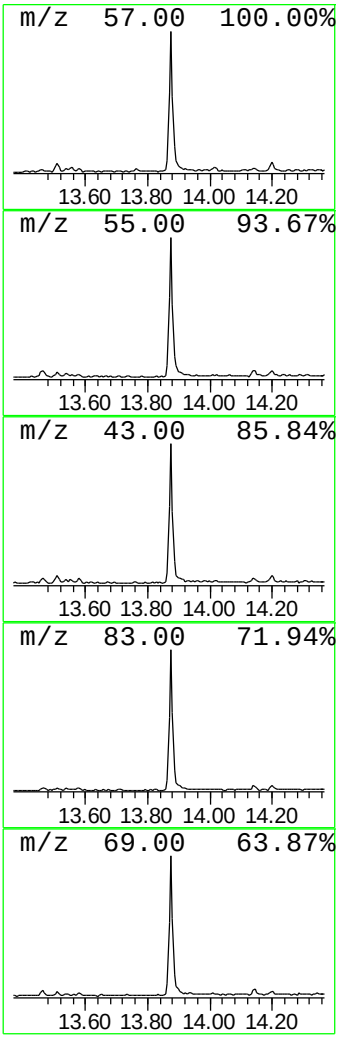
Peak Number 10 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	14.10 ng	852885	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
2	1-Docosene	308	C22H44	001599-67-3	94
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94





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Acq On : 6 Feb 2018 4:51
Operator : SJ/JU
Sample : J1454-06
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-SAN-6-EW(4-8)

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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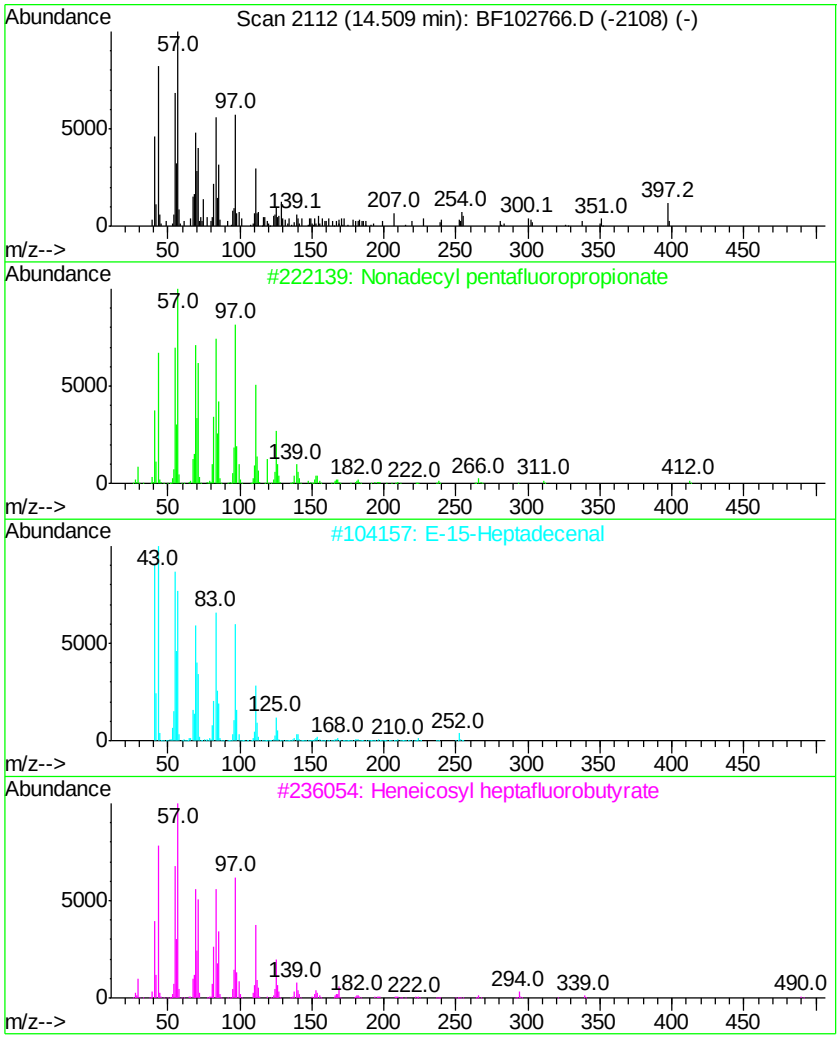
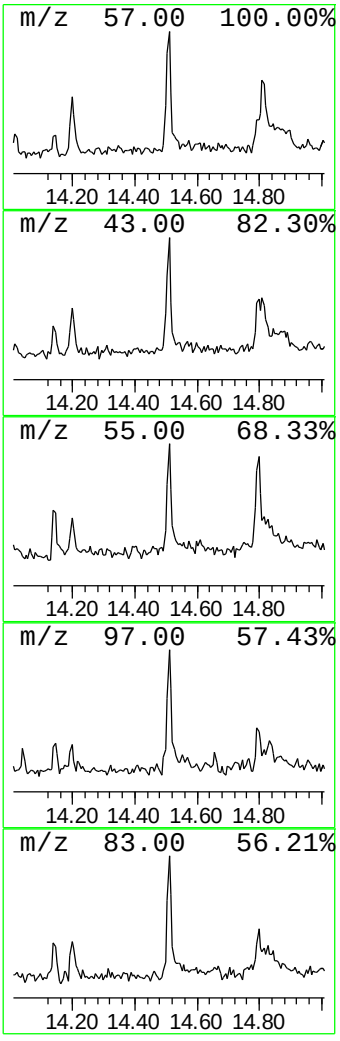
Peak Number 11 Nonadecyl pentafluoropropio... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.51	2.39 ng	144380	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	83
2	E-15-Heptadecenal	252	C17H32O	1000130-97-9	83
3	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	80
4	1-Octadecene	252	C18H36	000112-88-9	64
5	1-Heptacosanol	396	C27H56O	002004-39-9	58





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Data File : BF102766.D
Acq On : 6 Feb 2018 4:51
Operator : SJ/JU
Sample : J1454-06
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-SAN-6-EW(4-8)

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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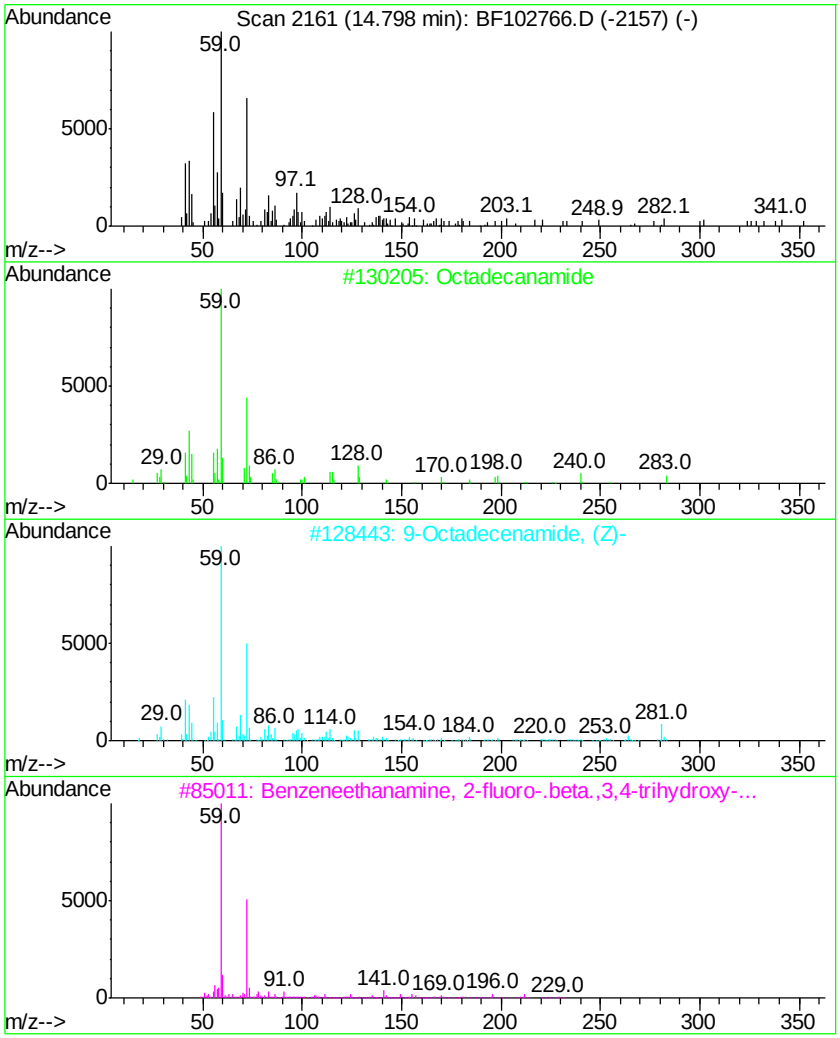
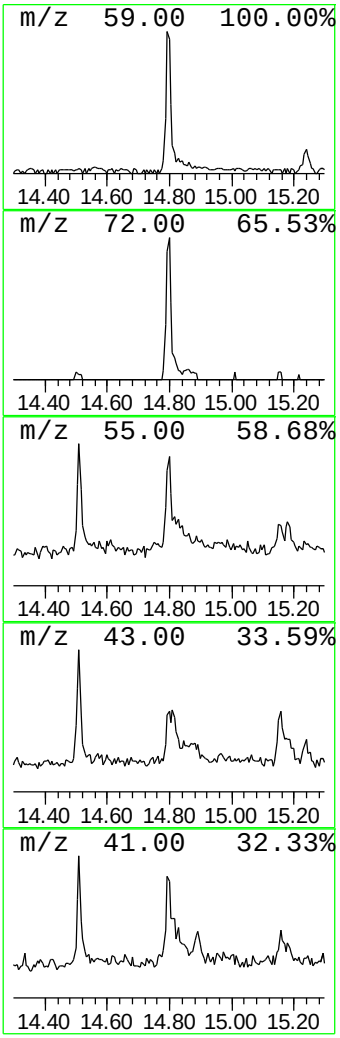
Peak Number 12 Octadecanamide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	3.23 ng	175458	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanamide	283	C18H37NO	000124-26-5	78
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	58
3	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	53
4	5-Fluoroorotyl-N,N-dimethylhydra...	216	C7H9FN4O3	1000227-24-4	43
5	Tetradecanamide	227	C14H29NO	000638-58-4	43





Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102766.D
Acq On : 6 Feb 2018 4:51
Operator : SJ/JU
Sample : J1454-06
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-SAN-6-EW(4-8)

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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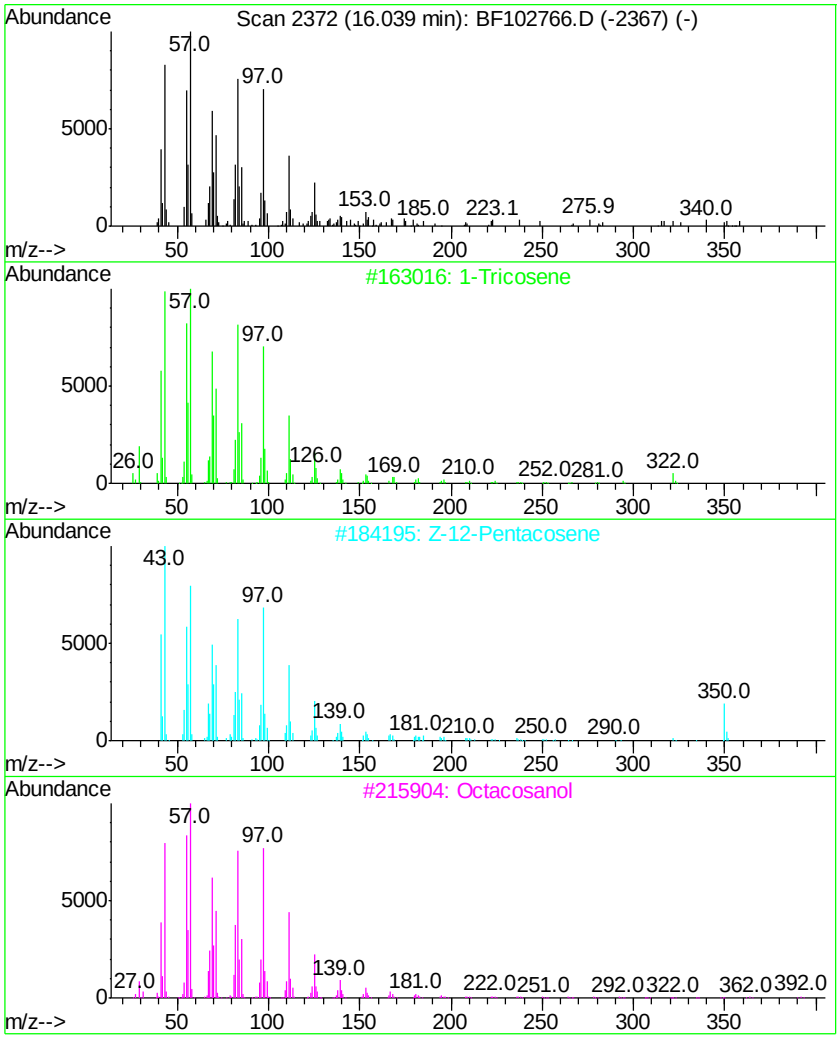
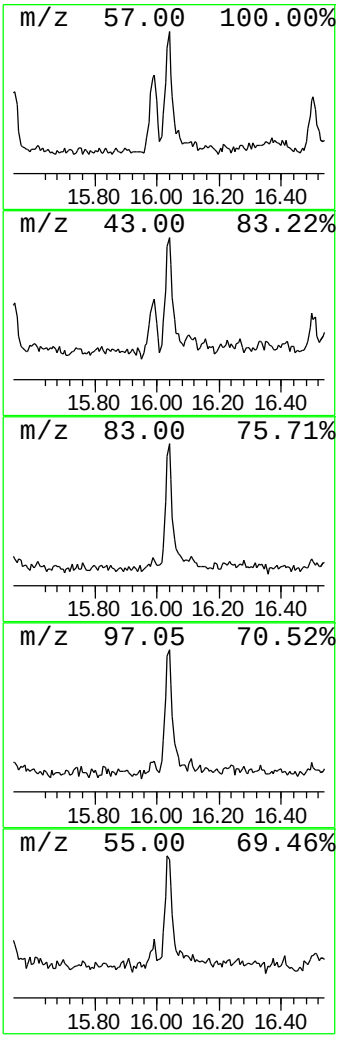
Peak Number 13 1-Tricosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.04	3.68 ng	200126	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	95
2	Z-12-Pentacosene	350	C25H50	1000131-09-4	95
3	Octacosanol	410	C28H58O	000557-61-9	91
4	9-Tricosene, (Z)-	322	C23H46	027519-02-4	91
5	Octacosyl acetate	452	C30H60O2	018206-97-8	91





Tentatively Identified Compound (LSC) summary

Data Path : U:\HPCHEM1\BNA_F\DATA\BF020518\
Data File : BF102766.D
Acq On : 6 Feb 2018 4:51
Operator : SJ/JU
Sample : J1454-06
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-SAN-6-EW(4-8)

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...	2.19	10.7	ng	765823	1	6.88	1425820	20.0
2-Pentanone, 4-hy...	5.12	2.7	ng	194692	1	6.88	1425820	20.0
unknown6.65	6.65	69.6	ng	4960360	1	6.88	1425820	20.0
Benzene, 1,2,3-tr...	6.70	3.0	ng	213413	1	6.88	1425820	20.0
Benzene, 1,2-diet...	7.20	2.2	ng	154084	1	6.88	1425820	20.0
Hexadecane	10.82	2.3	ng	186714	4	11.40	1624620	20.0
n-Hexadecanoic acid	11.93	7.3	ng	588673	4	11.40	1624620	20.0
Pentafluoropropio...	13.87	14.1	ng	852885	5	14.04	1209550	20.0
Nonadecyl pentafl...	14.51	2.4	ng	144380	5	14.04	1209550	20.0
Octadecanamide	14.80	3.2	ng	175458	6	15.52	1087360	20.0
1-Tricosene	16.04	3.7	ng	200126	6	15.52	1087360	20.0