LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071218\
Data File : BF107351.D
Acq On : 12 Jul 2018 20:40
Operator : JU/SJ
Sample : J3927-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-RBR-200031

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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	5.166	477	481	492	rBV	143516	186073	14.72%	1.500%
2	5.572	547	550	570	rBV	1061025	1143199	90.44%	9.213%
3	6.578	717	721	739	rBV	1093793	1151888	91.12%	9.283%
4	6.707	739	743	752	rVB	1240624	1129398	89.34%	9.102%
5	6.931	777	781	788	rBB	433495	381171	30.15%	3.072%
6	7.084	803	807	811	rBV	1020994	923972	73.09%	7.446%
7	7.495	873	877	887	rBV	716934	715241	56.58%	5.764%
8	8.213	995	999	1020	rBV	487482	459290	36.33%	3.701%
9	9.289	1178	1182	1190	rBV	1332970	1199084	94.86%	9.663%
10	9.683	1244	1249	1256	rBV	179567	159242	12.60%	1.283%
11	9.978	1295	1299	1310	rVB	462458	424962	33.62%	3.425%
12	10.777	1431	1435	1443	rBV	638244	627752	49.66%	5.059%
13	11.095	1484	1489	1494	rBV3	17825	18442	1.46%	0.149%
14	11.477	1550	1554	1557	rBV	458357	433057	34.26%	3.490%
15	11.901	1623	1626	1629	rBV2	13431	14740	1.17%	0.119%
16	12.095	1655	1659	1661	rBV4	9448	13701	1.08%	0.110%
17	12.266	1684	1688	1693	rBV5	10047	16996	1.34%	0.137%
18	12.477	1721	1724	1727	rVB2	17738	17478	1.38%	0.141%
19	12.530	1730	1733	1737	rVB3	16936	16244	1.29%	0.131%
20	12.695	1758	1761	1766	rVB	93807	82931	6.56%	0.668%
21	12.907	1794	1797	1798	rBV2	23132	19179	1.52%	0.155%
22	12.930	1798	1801	1804	rVB	99616	87159	6.89%	0.702%
23	13.060	1819	1823	1826	rBV	1380493	1264110	100.00%	10.187%
24	13.260	1854	1857	1861	rVB	39065	33983	2.69%	0.274%
25	13.513	1898	1900	1906	rVB5	12942	17931	1.42%	0.145%
26	13.601	1913	1915	1918	rBV	37979	34616	2.74%	0.279%
27	13.883	1960	1963	1965	rBV	14232	14982	1.19%	0.121%
28	13.936	1969	1972	1978	rVV3	78016	119530	9.46%	0.963%
29	14.071	1993	1995	1999	rVB	20468	19676	1.56%	0.159%
30	14.136	2001	2006	2009	rBV	540988	575393	45.52%	4.637%
31	14.160	2009	2010	2015	rVB	58083	39815	3.15%	0.321%
32	14.201	2015	2017	2022	rBV5	11493	16488	1.30%	0.133%
33	14.248	2022	2025	2029	rBV2	59657	67910	5.37%	0.547%
34	14.560	2074	2078	2081	rBV	81180	87377	6.91%	0.704%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071218\
Data File : BF107351.D
Acq On : 12 Jul 2018 20:40
Operator : JU/SJ
Sample : J3927-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-RBR-200031

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.871	2128	2131	2136	rBV	61231	65101	5.15%	0.525%
36	14.954	2141	2145	2150	rVB2	93923	110803	8.77%	0.893%
37	15.224	2186	2191	2198	rVB2	100256	171706	13.58%	1.384%
38	15.536	2242	2244	2250	rVB	21639	24227	1.92%	0.195%
39	15.618	2252	2258	2262	rBV2	55942	101431	8.02%	0.817%
40	15.671	2262	2267	2272	rBV	253756	333480	26.38%	2.687%
41	16.077	2331	2336	2341	rVB	42073	63800	5.05%	0.514%
42	16.607	2423	2426	2430	rVB3	17386	25118	1.99%	0.202%

Sum of corrected areas: 12408676

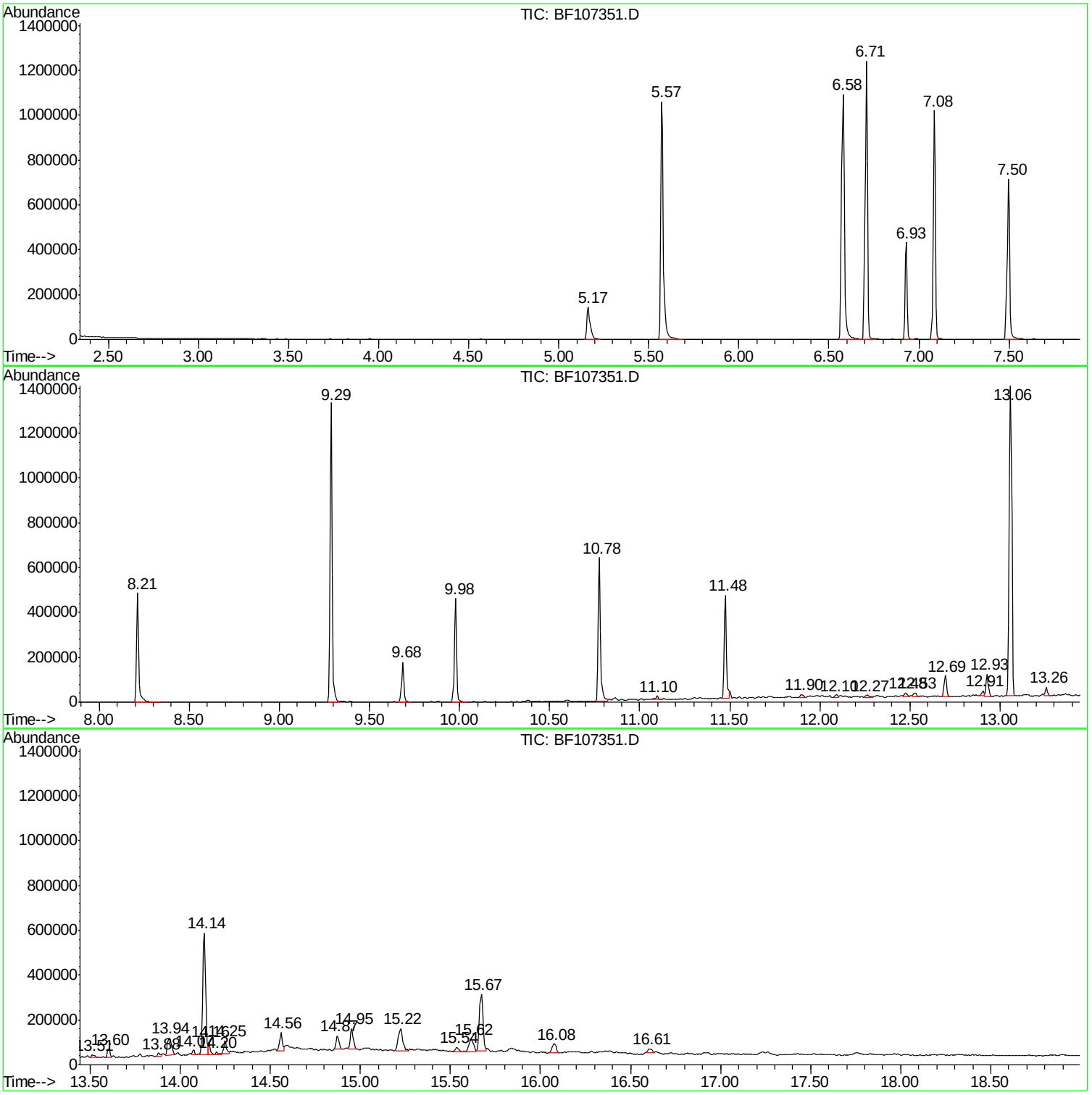
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071218\
Data File : BF107351.D
Acq On : 12 Jul 2018 20:40
Operator : JU/SJ
Sample : J3927-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CS-RBR-200031

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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:\SVOASRV\HPCHEM1\BNA F\DATA\BF071218\
Data File : BF107351.D
Acq On : 12 Jul 2018 20:40
Operator : JU/SJ
Sample : J3927-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-RBR-200031

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

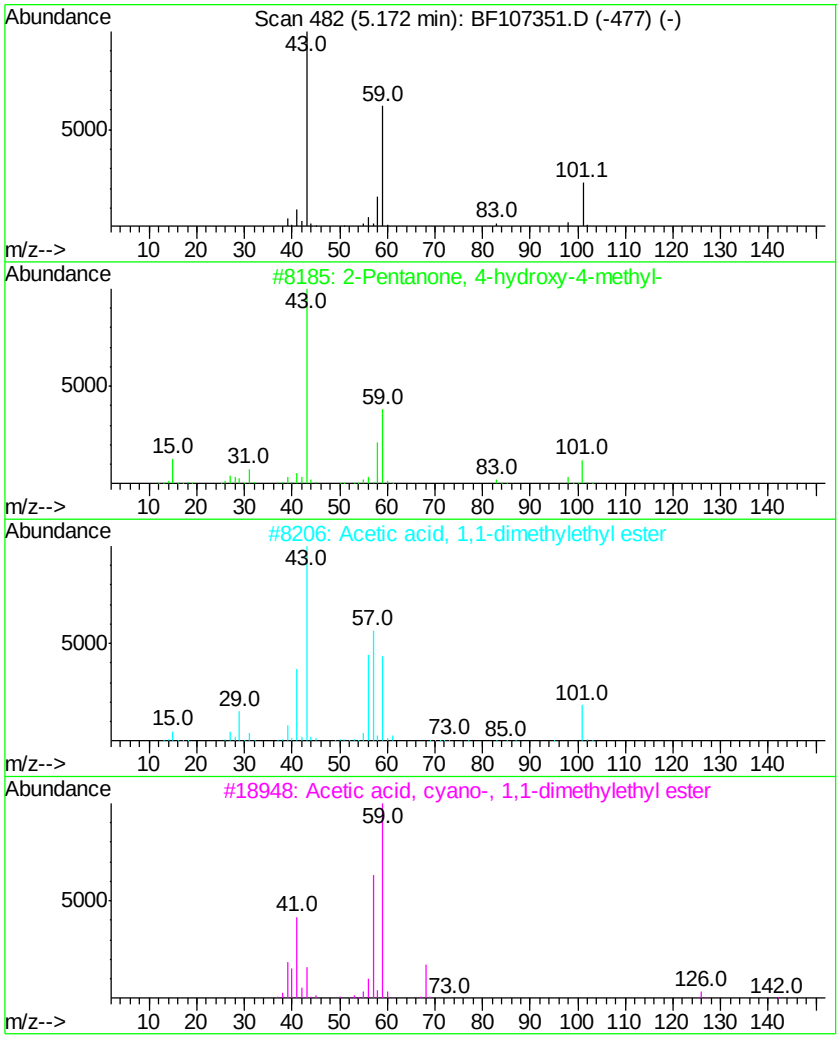
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

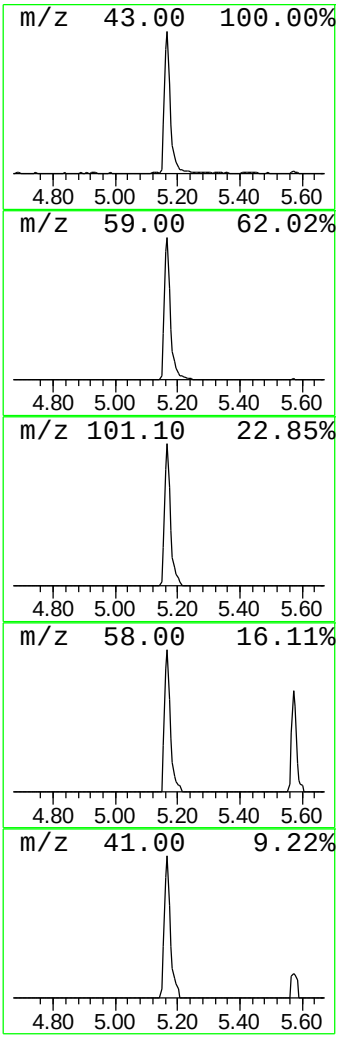
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	9.76 ng	186073	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071218\
Data File : BF107351.D
Acq On : 12 Jul 2018 20:40
Operator : JU/SJ
Sample : J3927-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-RBR-200031

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

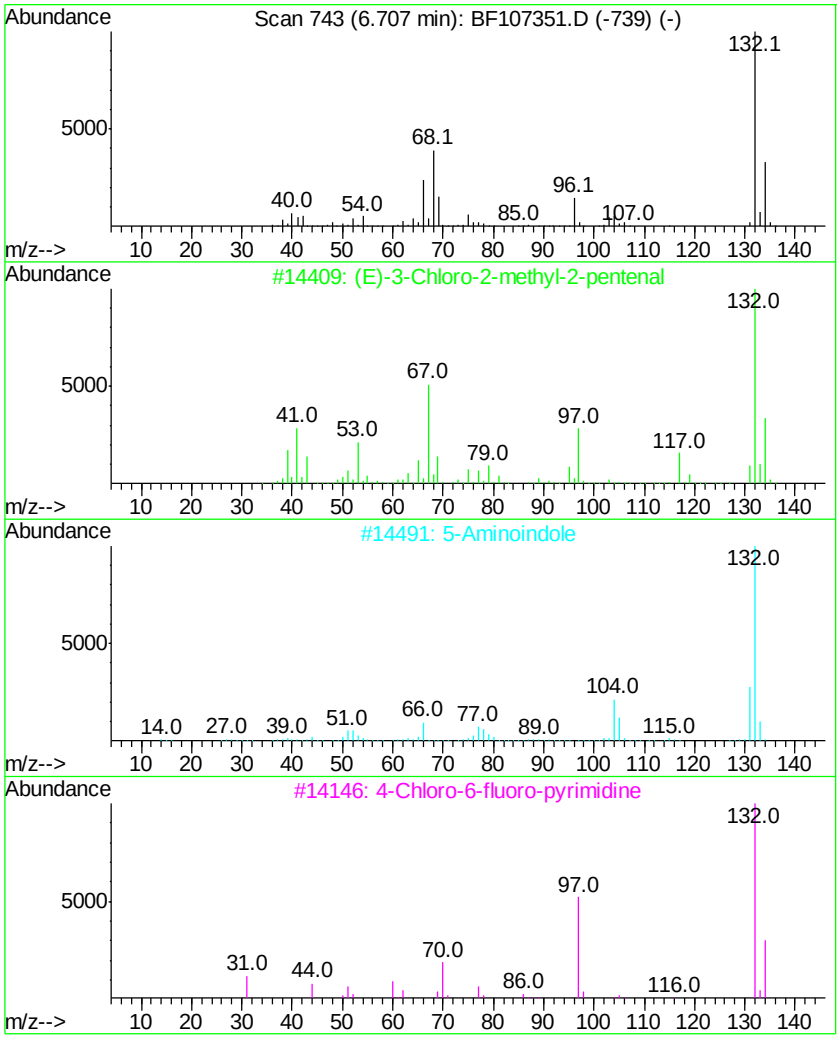
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

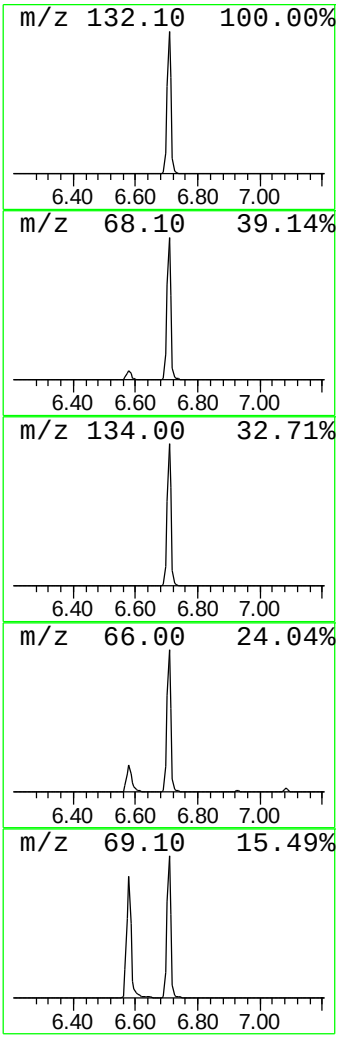
****

Peak Number 2 unknown6.71 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	59.26 ng	1129400	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071218\
Data File : BF107351.D
Acq On : 12 Jul 2018 20:40
Operator : JU/SJ
Sample : J3927-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-RBR-200031

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

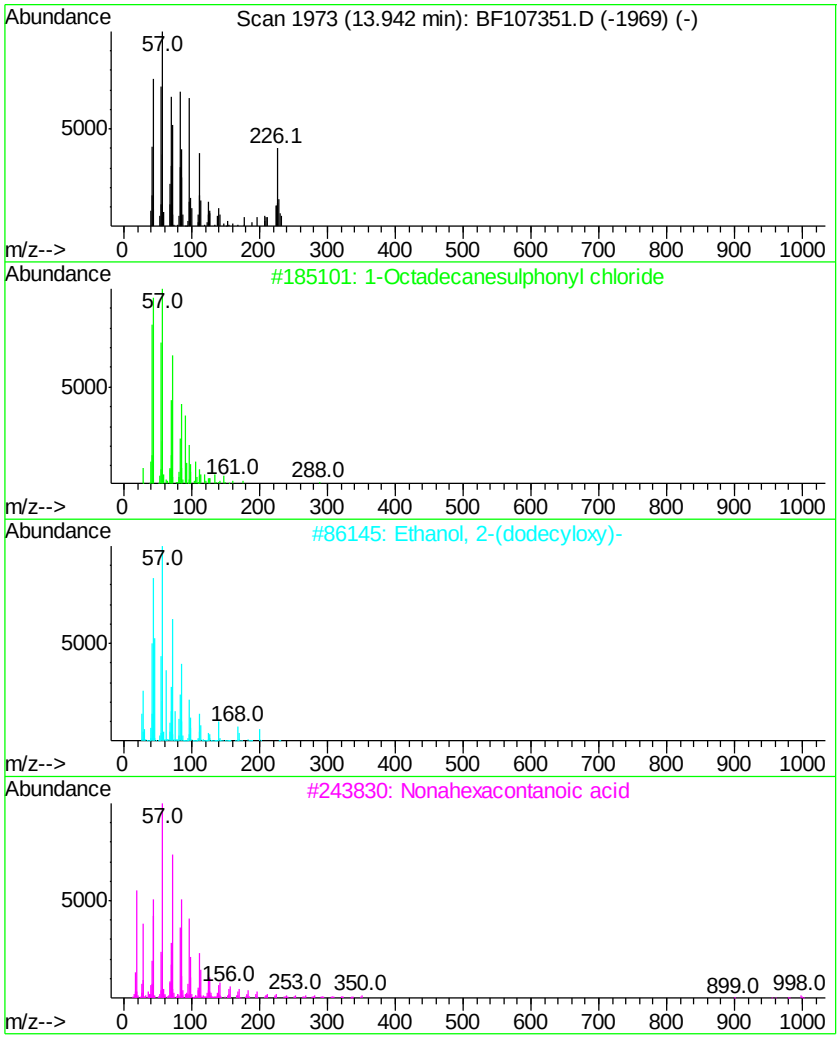
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

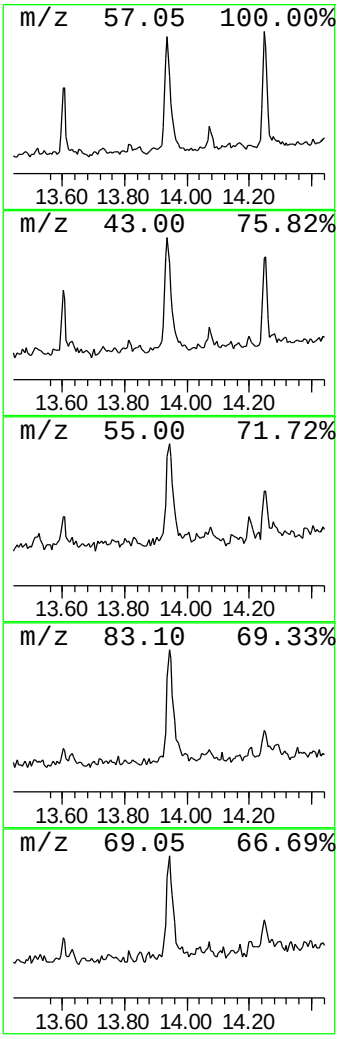
****

Peak Number 4 1-Octadecanesulphonyl chloride Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	4.15 ng	119530	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	68
2	Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	64
3	Nonahexacontanoic acid	999	C69H138O2	040710-32-5	52
4	Hexadecane	226	C16H34	000544-76-3	52
5	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	52





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071218\
Data File : BF107351.D
Acq On : 12 Jul 2018 20:40
Operator : JU/SJ
Sample : J3927-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-RBR-200031

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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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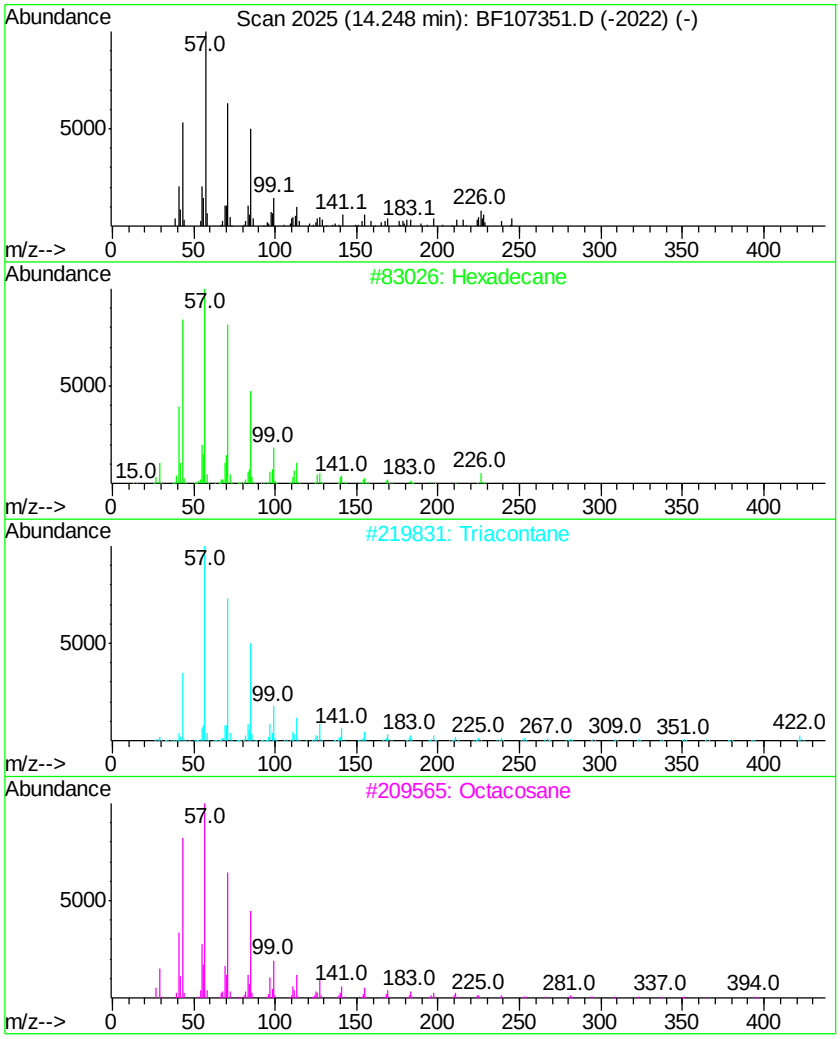
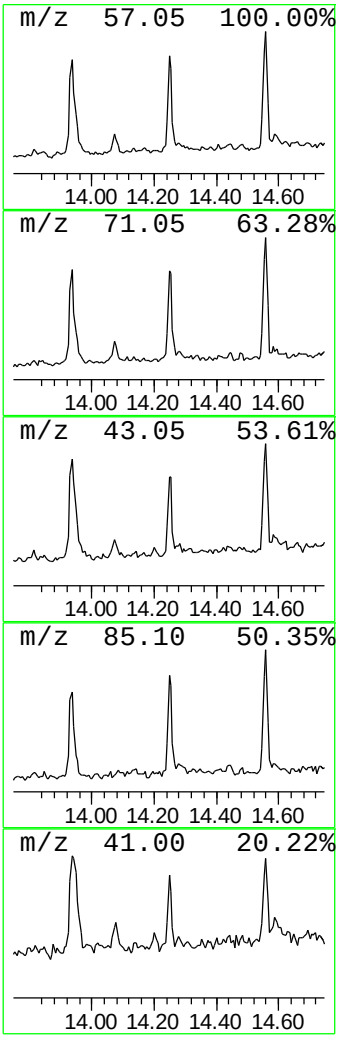
Peak Number 5 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.25	2.36 ng	67910	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	97
2	Triacontane	422	C30H62	000638-68-6	74
3	Octacosane	394	C28H58	000630-02-4	74
4	Heptadecane	240	C17H36	000629-78-7	74
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071218\
Data File : BF107351.D
Acq On : 12 Jul 2018 20:40
Operator : JU/SJ
Sample : J3927-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-RBR-200031

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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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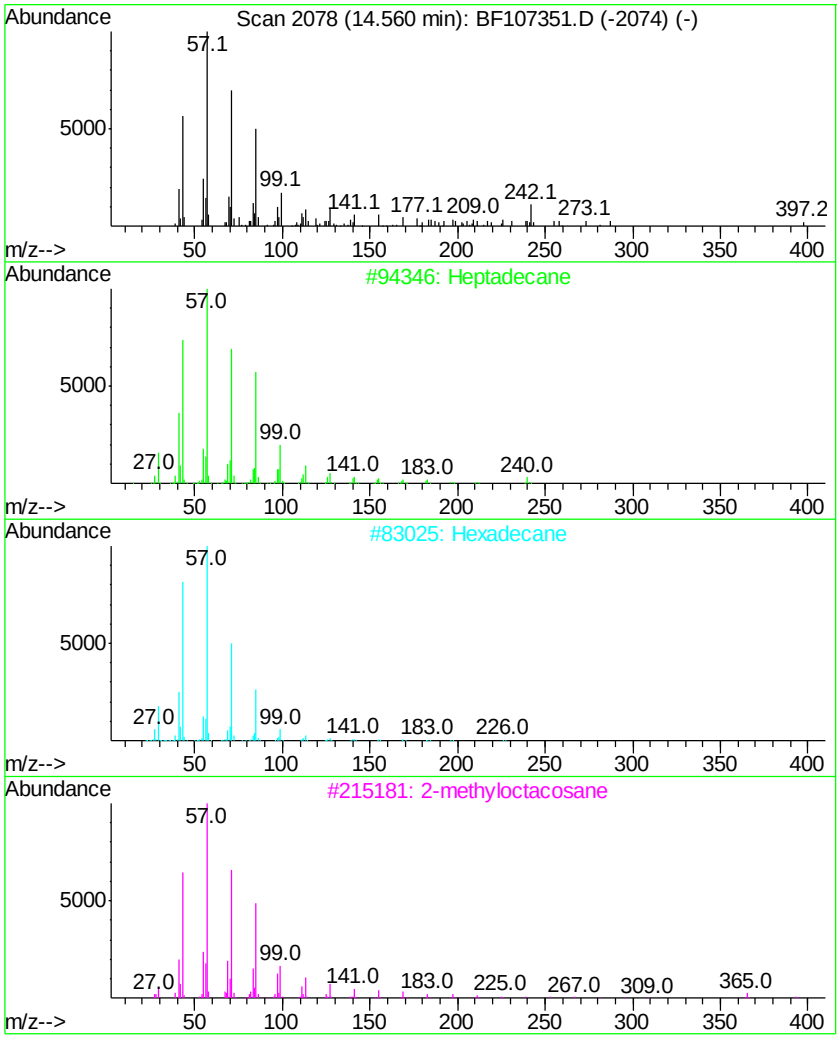
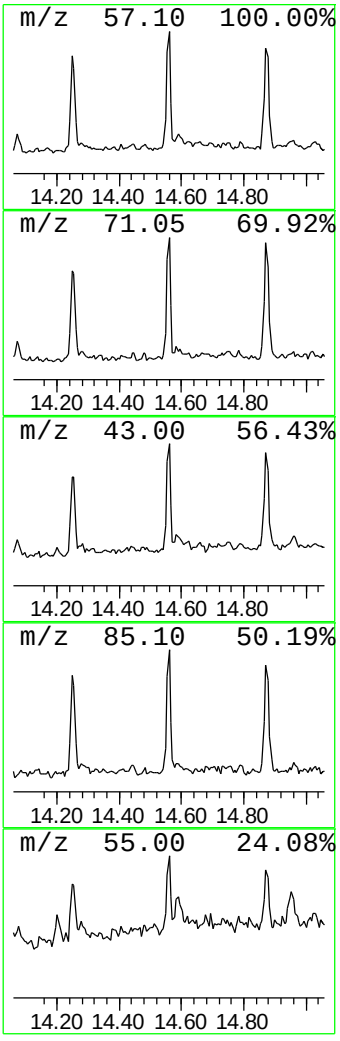
Peak Number 6 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	3.04 ng	87377	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	95
2	Hexadecane	226	C16H34	000544-76-3	95
3	2-methyloctacosane	408	C29H60	1000376-72-8	87
4	Docosane	310	C22H46	000629-97-0	87
5	Hexacosane	366	C26H54	000630-01-3	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071218\
Data File : BF107351.D
Acq On : 12 Jul 2018 20:40
Operator : JU/SJ
Sample : J3927-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-RBR-200031

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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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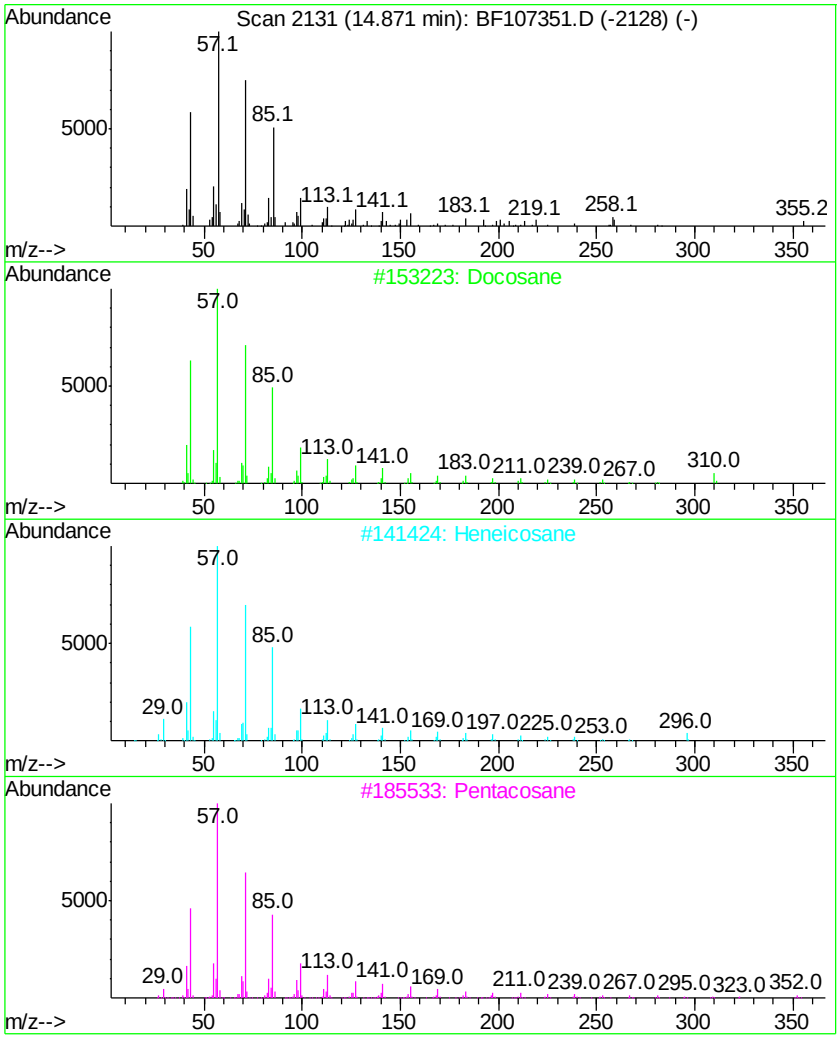
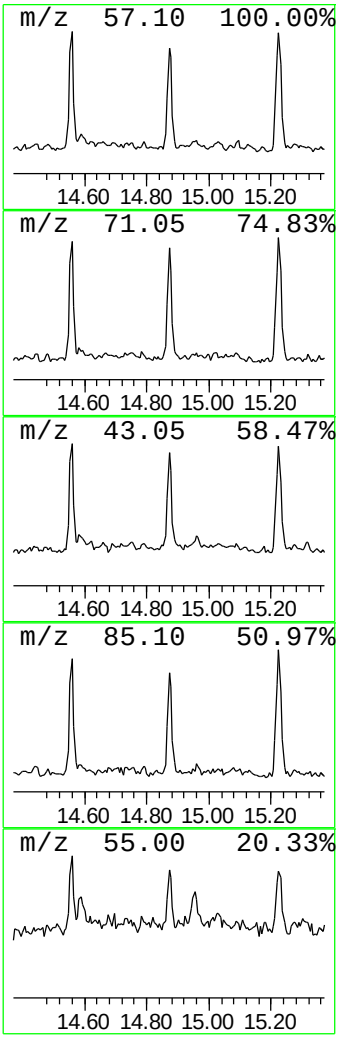
Peak Number 7 Docosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	2.26 ng	65101	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Pentacosane	352	C25H52	000629-99-2	90
4	Octadecane	254	C18H38	000593-45-3	90
5	Eicosane	282	C20H42	000112-95-8	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071218\
Data File : BF107351.D
Acq On : 12 Jul 2018 20:40
Operator : JU/SJ
Sample : J3927-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-RBR-200031

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

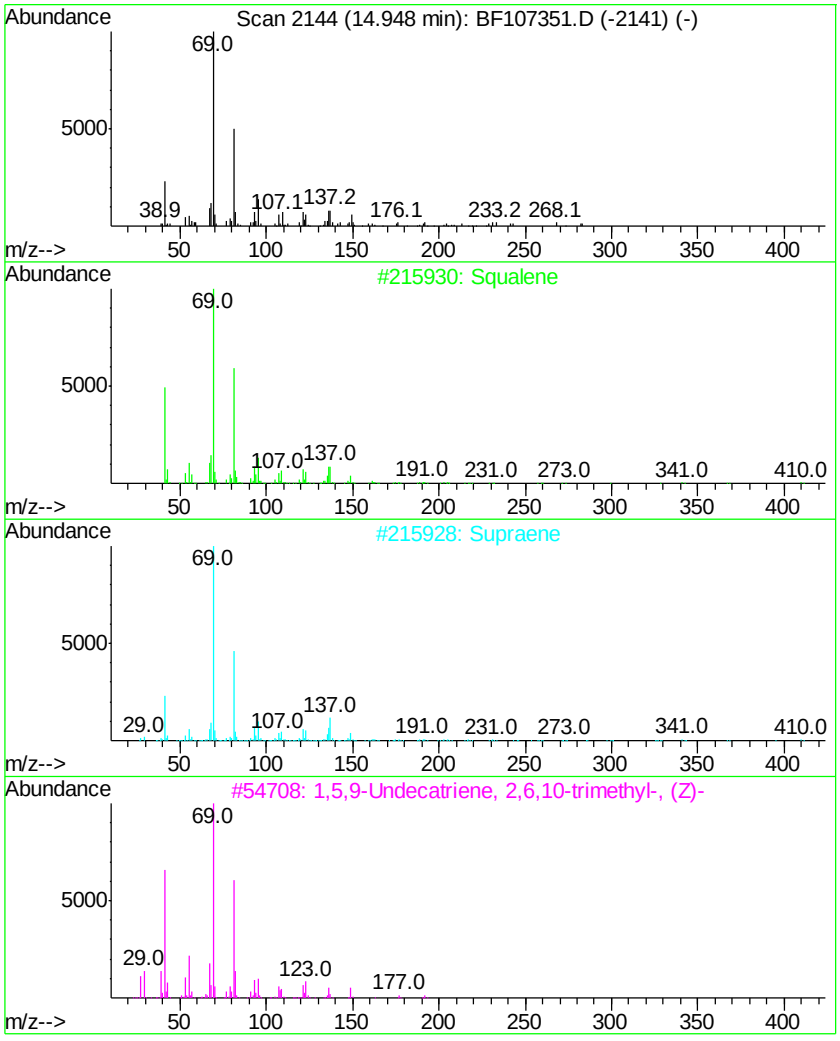
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

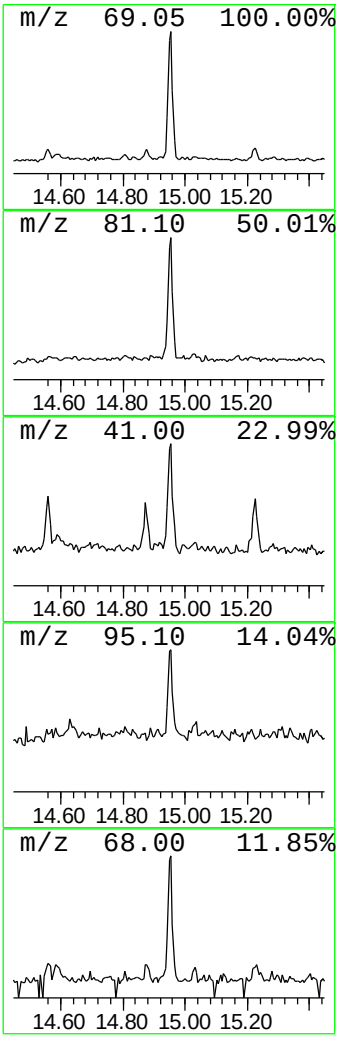
****

Peak Number 8 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	6.65 ng	110803	Perylene-d12	15.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	90
2	Supraene	410	C30H50	007683-64-9	87
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72
4	trans-Farnesol	222	C15H26O	000106-28-5	59
5	5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	53





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071218\
Data File : BF107351.D
Acq On : 12 Jul 2018 20:40
Operator : JU/SJ
Sample : J3927-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-RBR-200031

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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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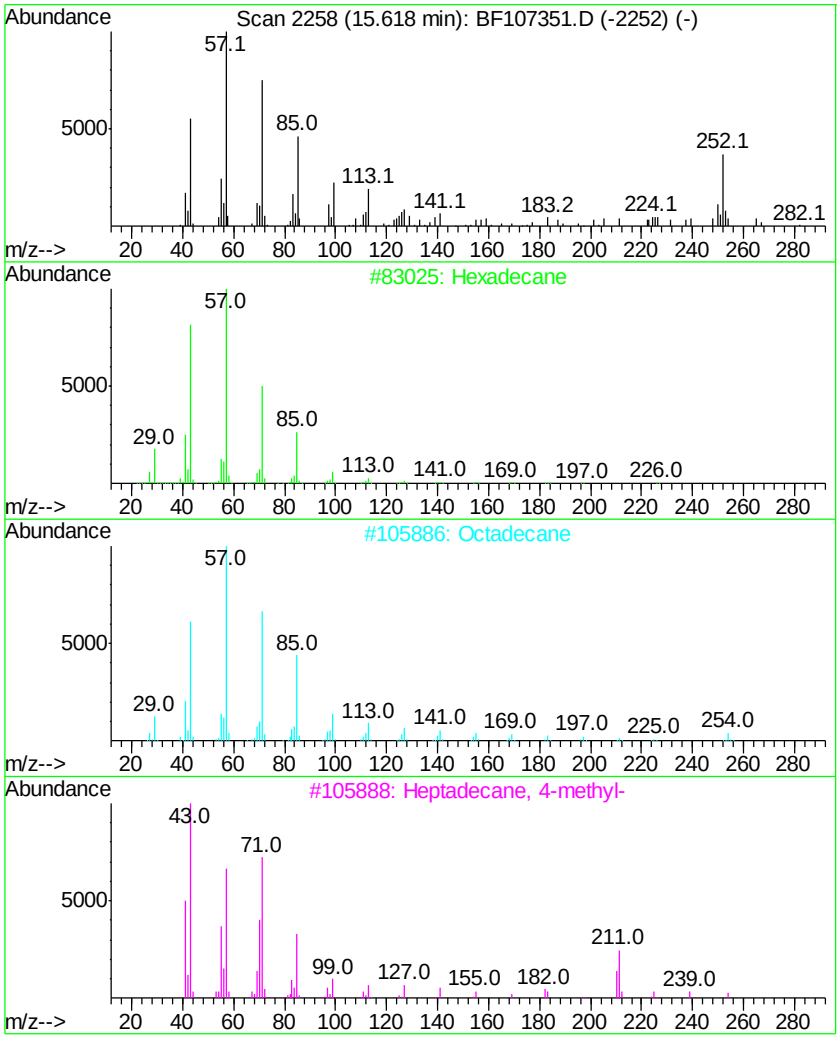
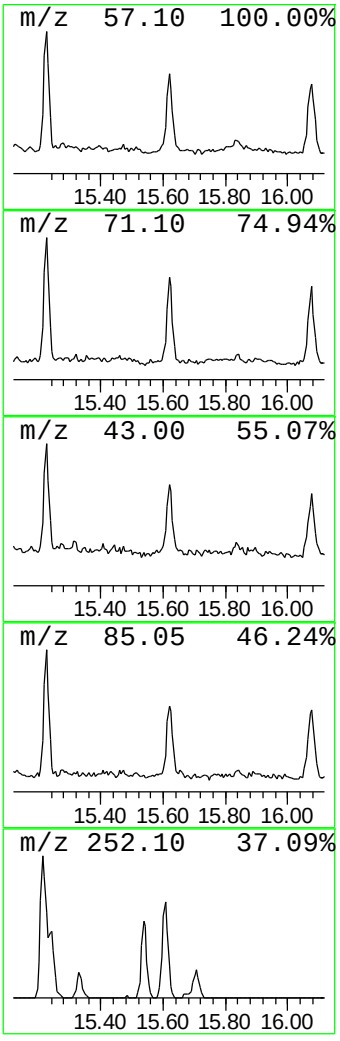
Peak Number 9 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.62	6.08 ng	101431	Perylene-d12	15.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	92
2	Octadecane	254	C18H38	000593-45-3	83
3	Heptadecane, 4-methyl-	254	C18H38	026429-11-8	64
4	Heneicosane	296	C21H44	000629-94-7	62
5	Pentacosane	352	C25H52	000629-99-2	62





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071218\
Data File : BF107351.D
Acq On : 12 Jul 2018 20:40
Operator : JU/SJ
Sample : J3927-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-RBR-200031

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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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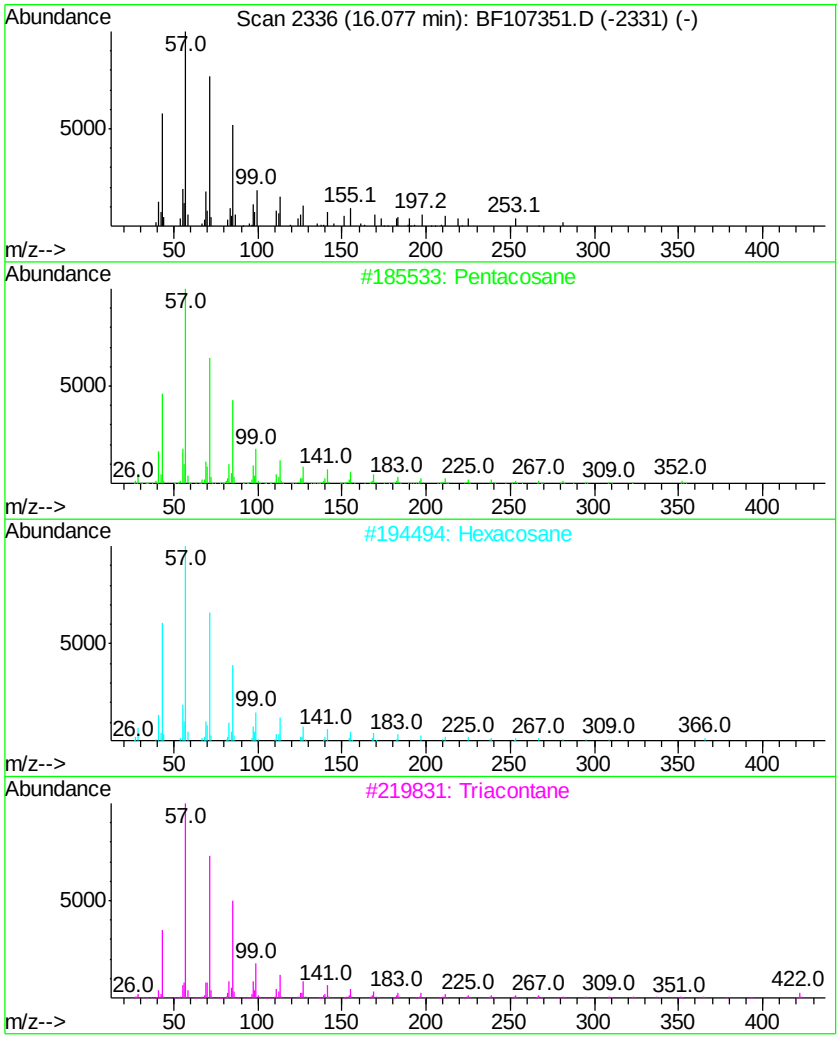
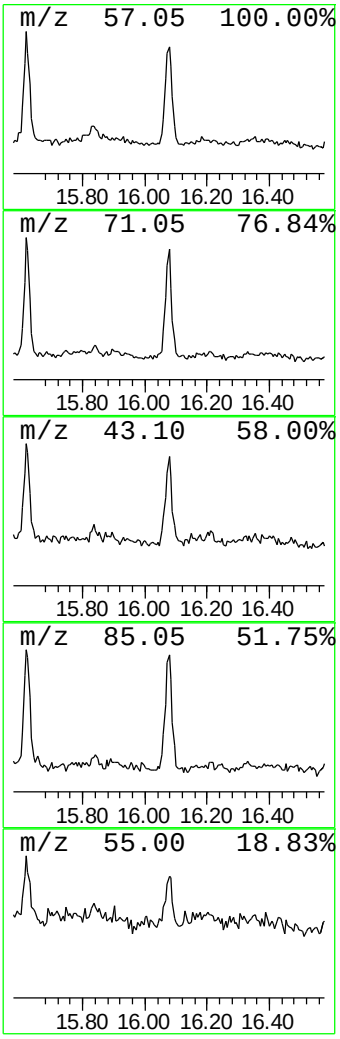
Peak Number 10 Pentacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.08	3.83 ng	63800	Perylene-d12	15.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Hentriacontane	437	C31H64	000630-04-6	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF071218\
Data File : BF107351.D
Acq On : 12 Jul 2018 20:40
Operator : JU/SJ
Sample : J3927-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-RBR-200031

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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...	5.17	9.8	ng	186073	1	6.93	381171	20.0
unknown6.71	6.71	59.3	ng	1129400	1	6.93	381171	20.0
1-Octadecanesulph...	13.94	4.2	ng	119530	5	14.14	575393	20.0
Hexadecane	14.25	2.4	ng	67910	5	14.14	575393	20.0
Heptadecane	14.56	3.0	ng	87377	5	14.14	575393	20.0
Docosane	14.87	2.3	ng	65101	5	14.14	575393	20.0
Squalene	14.95	6.7	ng	110803	6	15.67	333480	20.0
Octadecane	15.62	6.1	ng	101431	6	15.67	333480	20.0
Pentacosane	16.08	3.8	ng	63800	6	15.67	333480	20.0