LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101618\
Data File : BF109905.D
Acq On : 16 Oct 2018 15:13
Operator : JU/SJ
Sample : J5526-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-4B-C-101518-2

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-BF101518.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	2.322	35	40	51	rVB	717531	942955	20.48%	1.947%
2	3.587	252	255	268	rBV	51042	109015	2.37%	0.225%
3	5.216	528	532	538	rVB	163357	187458	4.07%	0.387%
4	5.598	592	597	601	rBV	4445351	4473407	97.16%	9.238%
5	6.598	762	767	771	rBV	4633537	4604123	100.00%	9.508%
6	6.751	788	793	796	rBV	4673299	4582842	99.54%	9.464%
7	6.981	828	832	835	rBV	2072662	1590731	34.55%	3.285%
8	7.140	855	859	862	rVB	4118103	3618372	78.59%	7.473%
9	7.539	922	927	930	rBV	3102198	2834912	61.57%	5.855%
10	8.263	1046	1050	1053	rBV	2400655	1967480	42.73%	4.063%
11	9.333	1228	1232	1236	rBV	4575562	4247529	92.25%	8.772%
12	9.728	1295	1299	1302	rBV	569974	447487	9.72%	0.924%
13	10.022	1345	1349	1353	rVB	2082858	1710516	37.15%	3.533%
14	10.810	1479	1483	1487	rBV	2261068	1898371	41.23%	3.920%
15	11.510	1599	1602	1605	rBV	1508291	1411654	30.66%	2.915%
16	11.533	1605	1606	1611	rVV	249693	184150	4.00%	0.380%
17	11.586	1611	1615	1618	rVB	51869	52143	1.13%	0.108%
18	11.722	1634	1638	1640	rBV2	56034	62201	1.35%	0.128%
19	12.022	1685	1689	1691	rBV2	169144	195501	4.25%	0.404%
20	12.127	1703	1707	1709	rBV2	60088	57865	1.26%	0.120%
21	12.539	1774	1777	1779	rBV	192664	146658	3.19%	0.303%
22	12.727	1805	1809	1814	rBV	620592	540866	11.75%	1.117%
23	12.804	1818	1822	1828	rVV3	122508	183095	3.98%	0.378%
24	12.957	1841	1848	1854	rBV	493566	534927	11.62%	1.105%
25	13.098	1868	1872	1875	rBV	3742193	3131477	68.01%	6.467%
26	13.174	1881	1885	1889	rBV3	32532	61069	1.33%	0.126%
27	13.286	1901	1904	1907	rVB	90375	77312	1.68%	0.160%
28	13.351	1912	1915	1918	rBV	61277	50011	1.09%	0.103%
29	13.392	1918	1922	1925	rBV2	51221	54508	1.18%	0.113%
30	13.792	1987	1990	1995	rVB	52464	64641	1.40%	0.133%
31	13.974	2016	2021	2036	rBV6	406222	722304	15.69%	1.492%
32	14.157	2047	2052	2055	rBV	2060765	2058569	44.71%	4.251%
33	14.180	2055	2056	2062	rVB	274421	210451	4.57%	0.435%
34	14.263	2068	2070	2074	rVB	67737	55648	1.21%	0.115%

LSC Area Percent Report

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Data File : BF109905.D
Acq On : 16 Oct 2018 15:13
Operator : JU/SJ
Sample : J5526-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-4B-C-101518-2

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-BF101518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.304	2074	2077	2082	rVB	118460	119681	2.60%	0.247%
36	14.610	2126	2129	2133	rBV	255298	248734	5.40%	0.514%
37	14.927	2180	2183	2190	rVB	220753	253364	5.50%	0.523%
38	15.010	2194	2197	2202	rVB	116249	112811	2.45%	0.233%
39	15.227	2230	2234	2237	rBV	265014	395695	8.59%	0.817%
40	15.286	2241	2244	2251	rVB	330829	408498	8.87%	0.844%
41	15.551	2286	2289	2295	rVB	166873	223445	4.85%	0.461%
42	15.615	2296	2300	2306	rBV	219122	280912	6.10%	0.580%
43	15.686	2307	2312	2323	rVV2	1592982	2293393	49.81%	4.736%
44	15.910	2348	2350	2354	rVB3	71995	77013	1.67%	0.159%
45	16.157	2387	2392	2397	rBV	322448	495168	10.75%	1.023%
46	16.704	2480	2485	2493	rVB	144123	263614	5.73%	0.544%
47	17.245	2573	2577	2586	rVB2	86624	179568	3.90%	0.371%

Sum of corrected areas: 48422144

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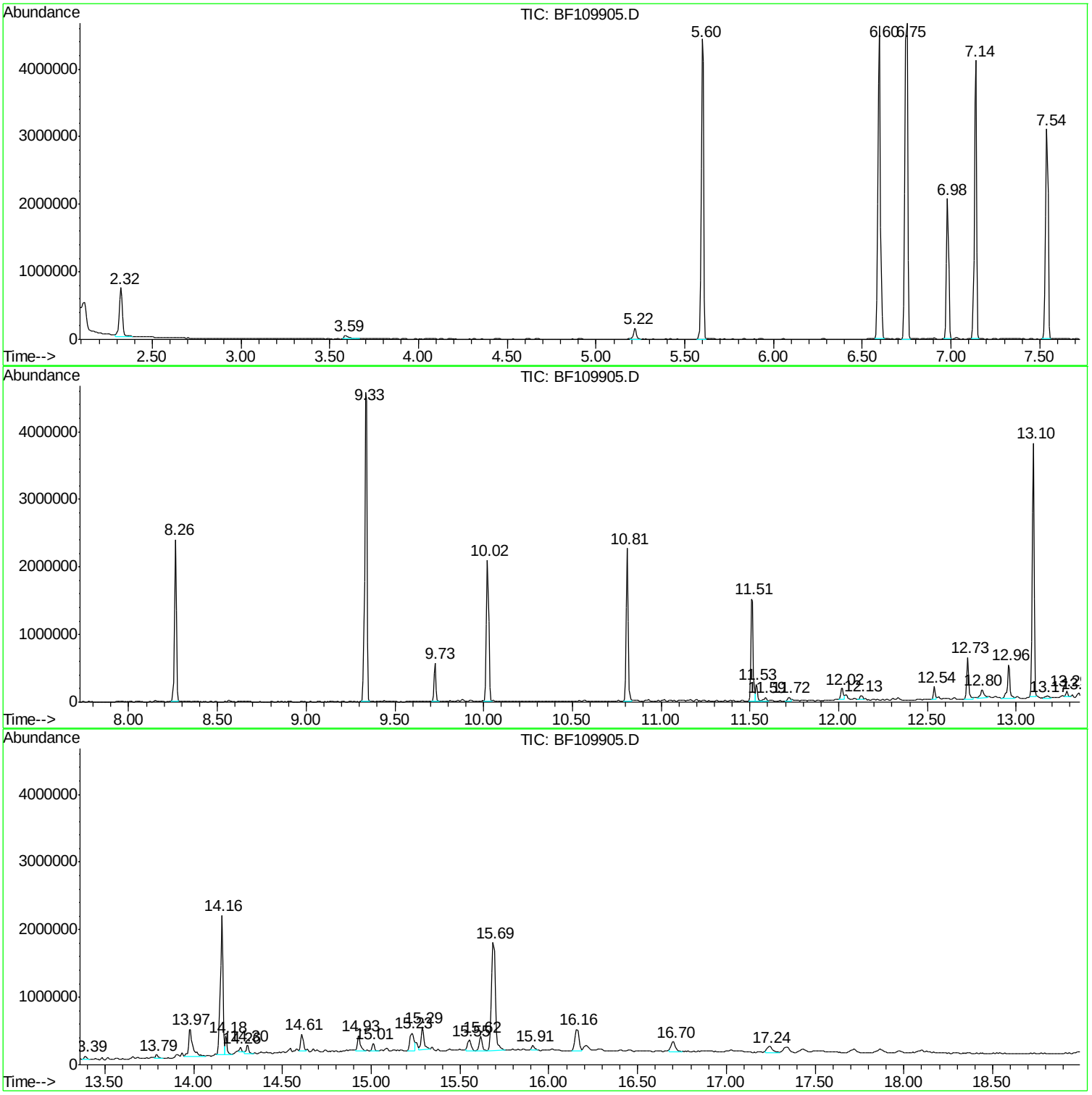
BNA_F
ClientSampleId :
SUP-4B-C-101518-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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

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Data File : BF109905.D
Acq On : 16 Oct 2018 15:13
Operator : JU/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : SUP-4B-C-101518-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

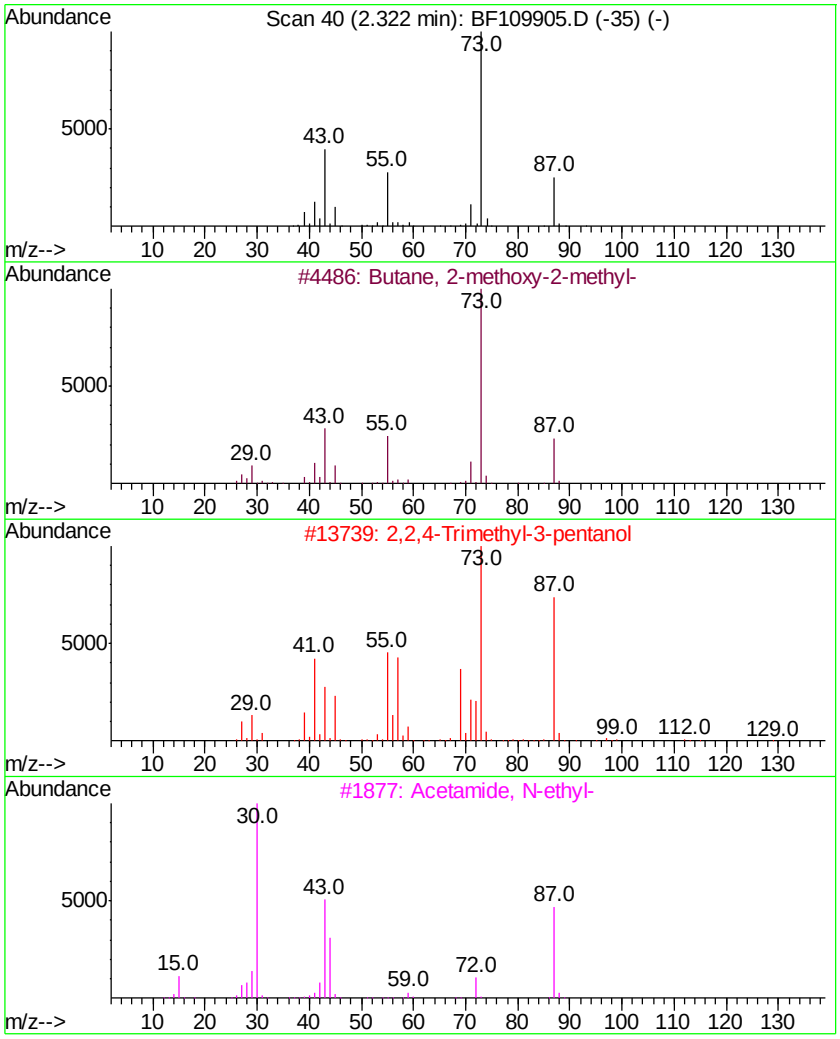
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

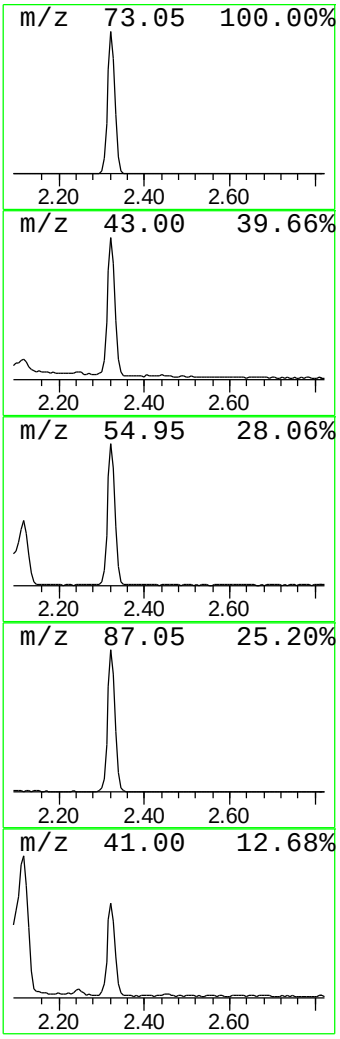
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.32	11.86 ng	942955	1,4-Dichlorobenzene-d4	6.98

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	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101618\
Data File : BF109905.D
Acq On : 16 Oct 2018 15:13
Operator : JU/SJ
Sample : J5526-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-4B-C-101518-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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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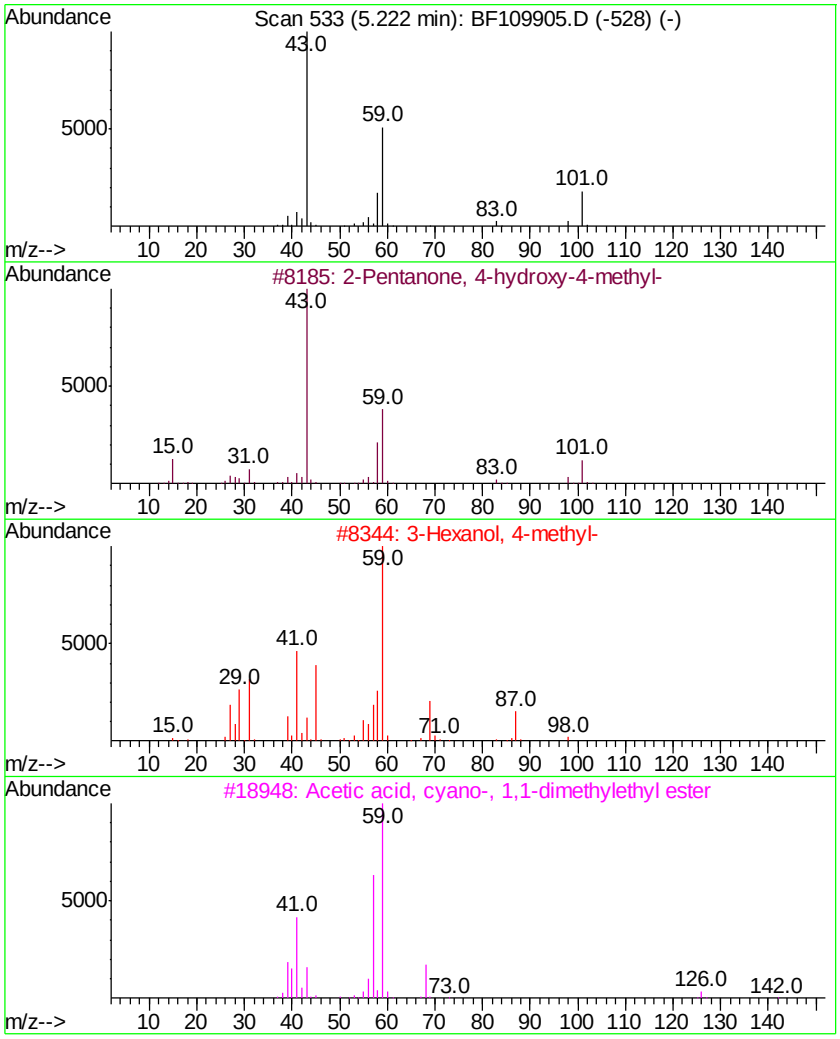
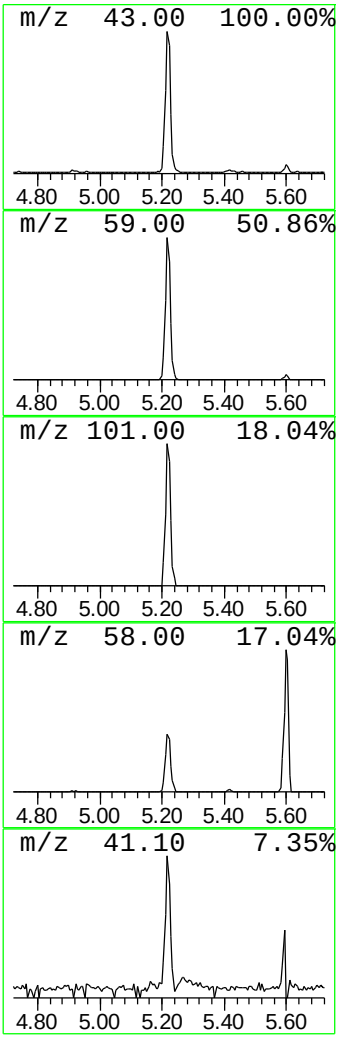
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	2.36 ng	187458	1,4-Dichlorobenzene-d4	6.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101618\
Data File : BF109905.D
Acq On : 16 Oct 2018 15:13
Operator : JU/SJ
Sample : J5526-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-4B-C-101518-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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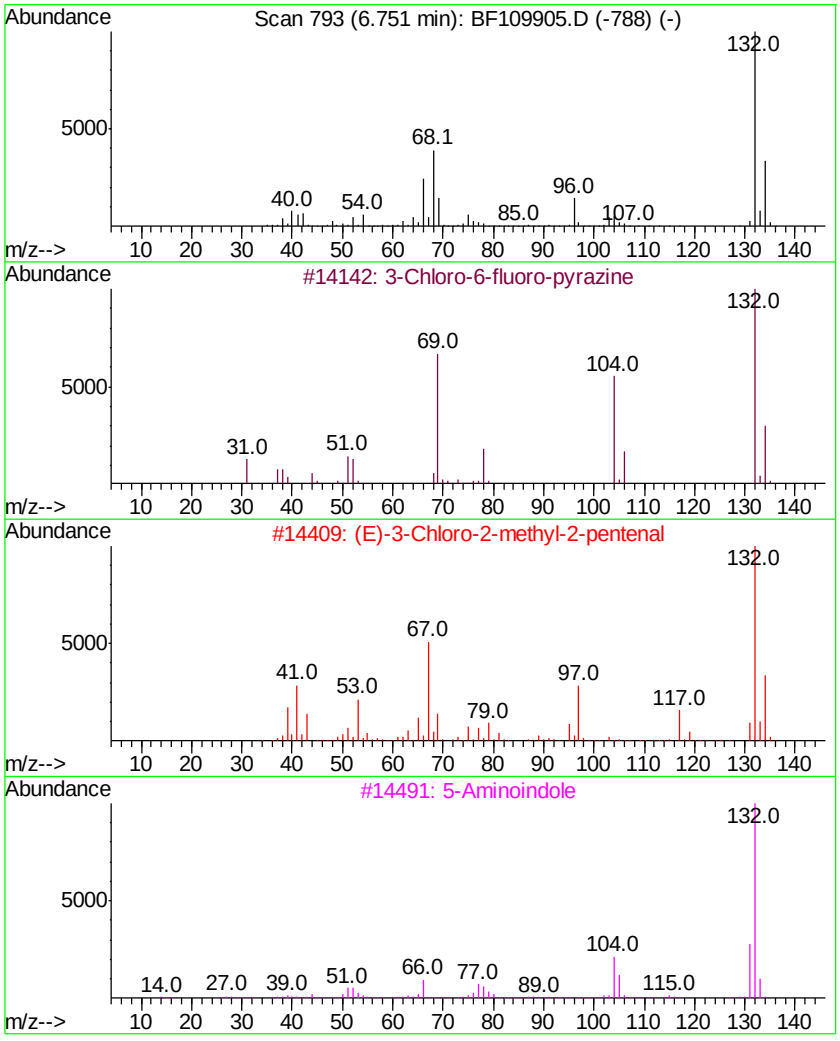
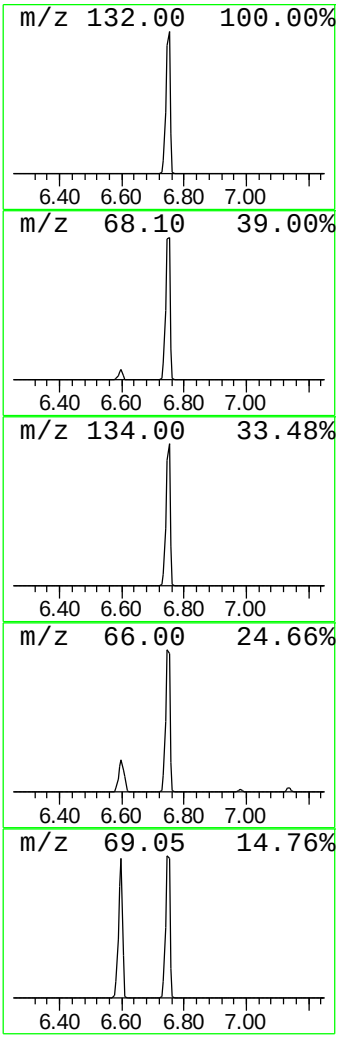
Peak Number 3 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	57.62 ng	4582840	1,4-Dichlorobenzene-d4	6.98

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	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-4B-C-101518-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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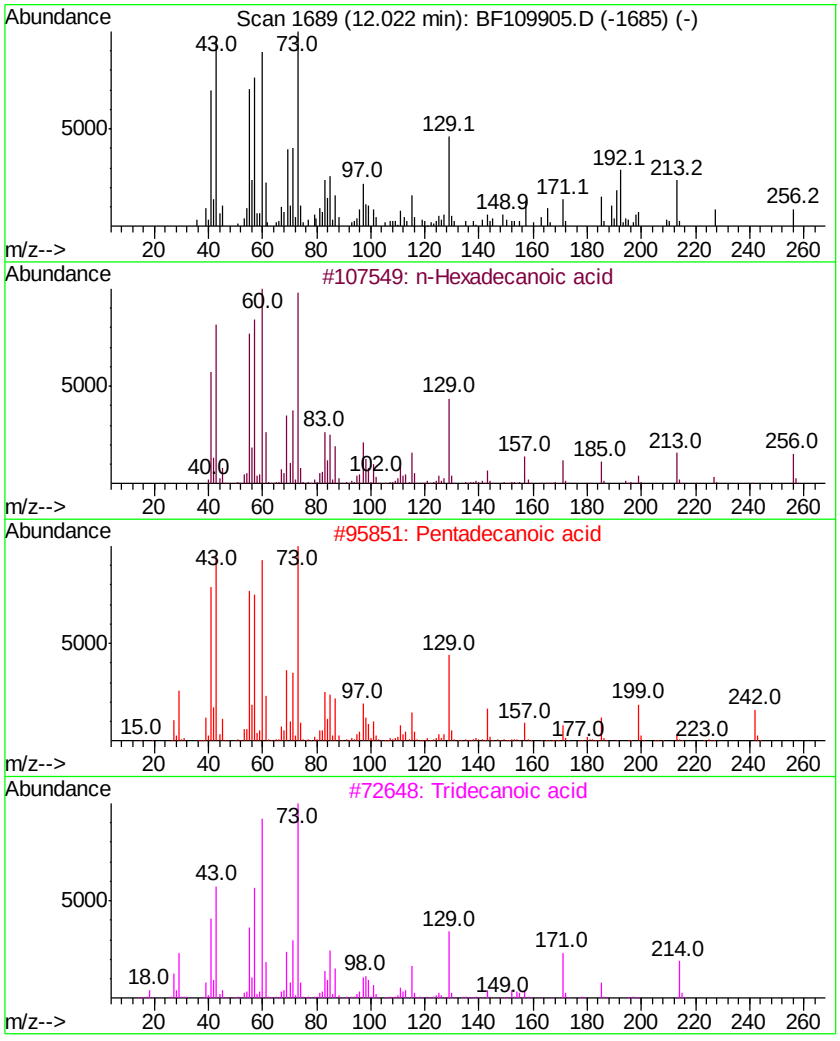
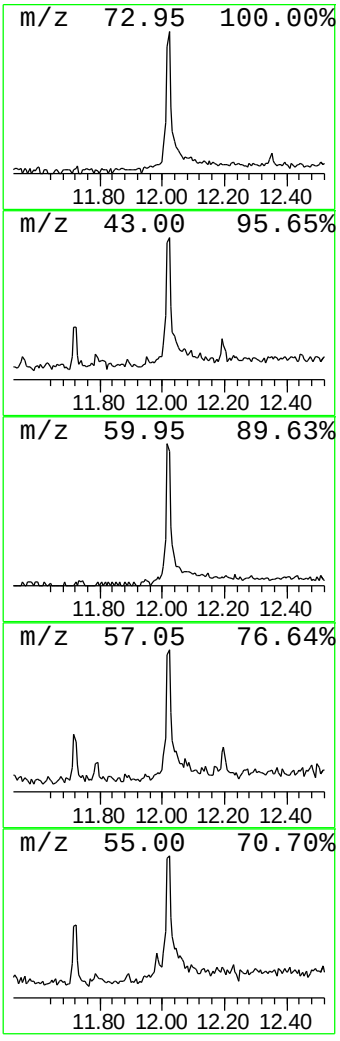
Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	2.77 ng	195501	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Undecanoic acid	186	C11H22O2	000112-37-8	62
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





Library Search Compound Report

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Data File : BF109905.D
Acq On : 16 Oct 2018 15:13
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Sample : J5526-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-4B-C-101518-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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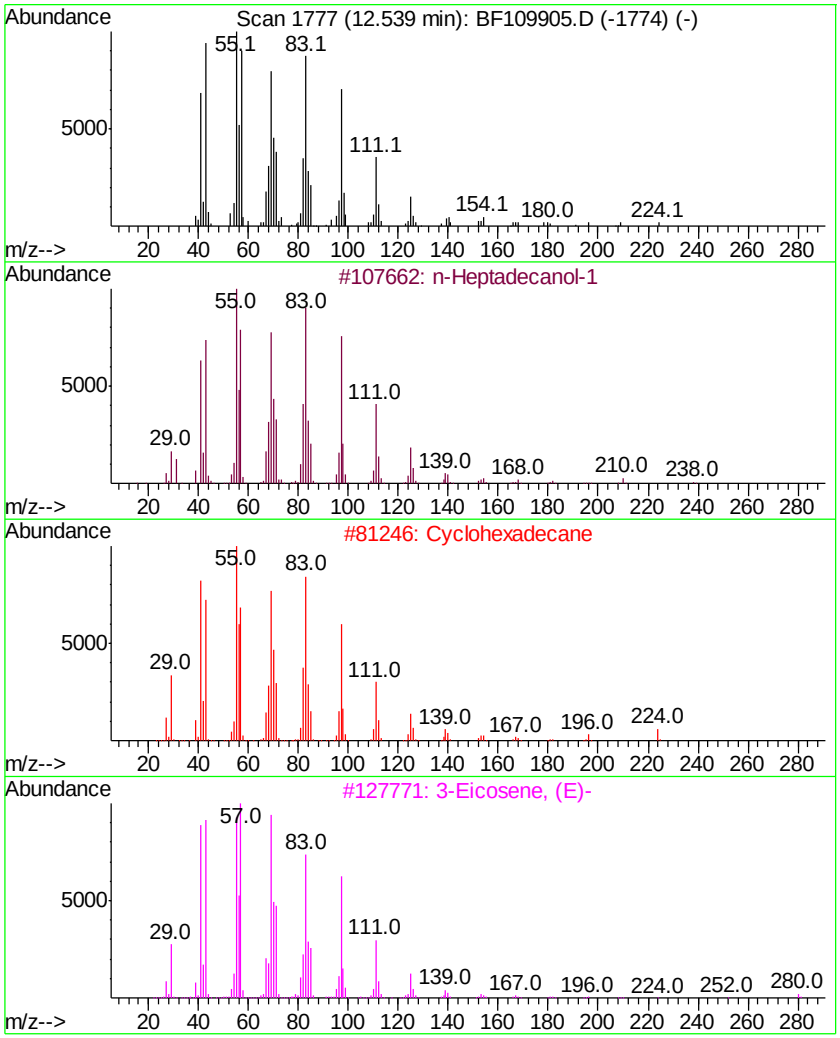
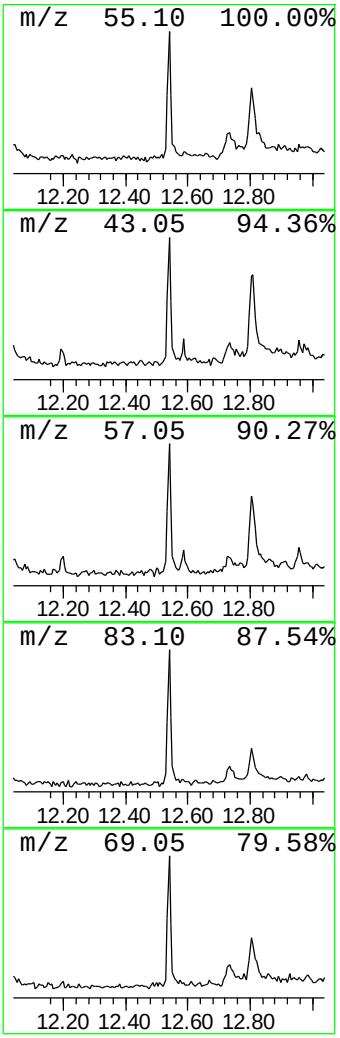
Peak Number 6 n-Heptadecanol-1 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.54	2.08 ng	146658	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Heptadecanol-1	256	C17H36O	001454-85-9	95
2	Cyclohexadecane	224	C16H32	000295-65-8	94
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	94
4	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
5	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	94





Library Search Compound Report

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Data File : BF109905.D
Acq On : 16 Oct 2018 15:13
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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-4B-C-101518-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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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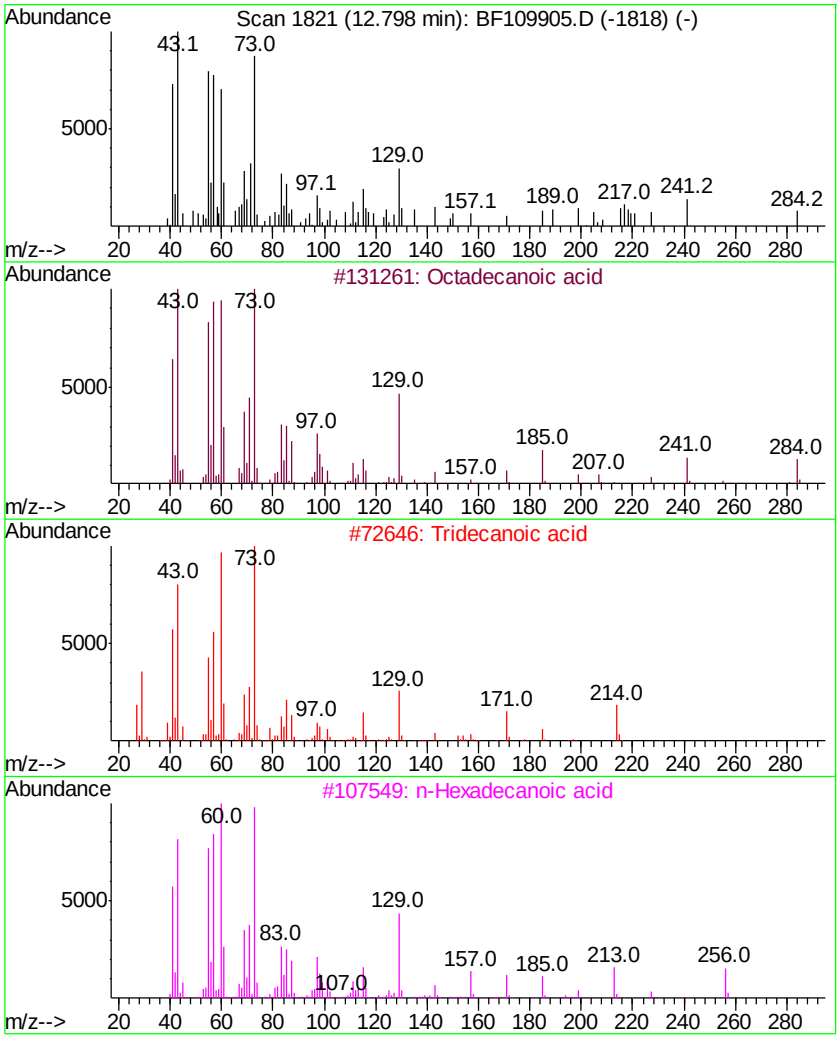
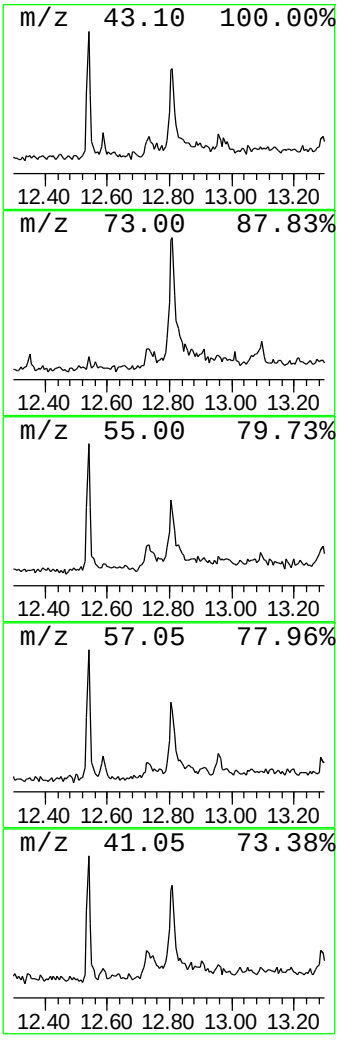
Peak Number 7 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	2.59 ng	183095	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	76
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
4	n-Decanoic acid	172	C10H20O2	000334-48-5	68
5	Undecanoic acid	186	C11H22O2	000112-37-8	60





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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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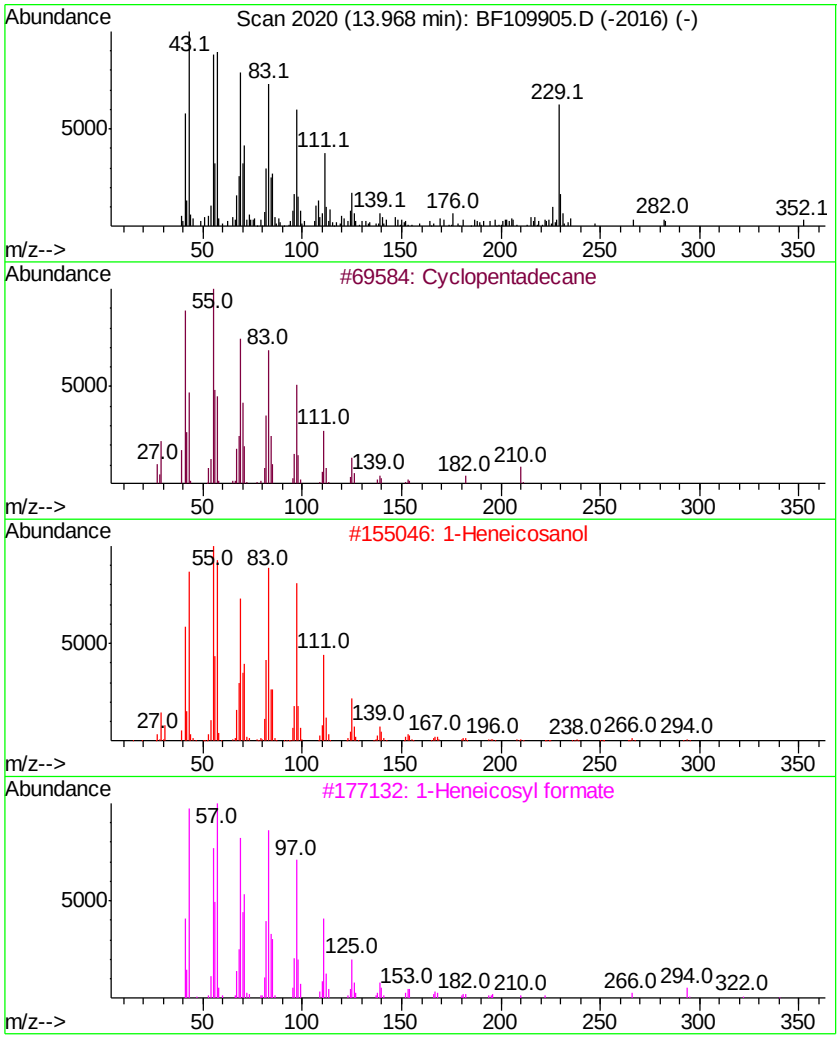
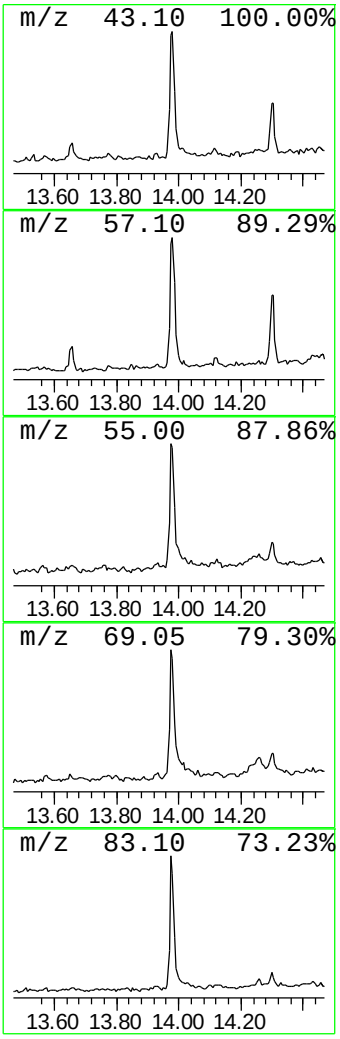
Peak Number 8 Cyclopentadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	7.02 ng	722304	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101618\
Data File : BF109905.D
Acq On : 16 Oct 2018 15:13
Operator : JU/SJ
Sample : J5526-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-4B-C-101518-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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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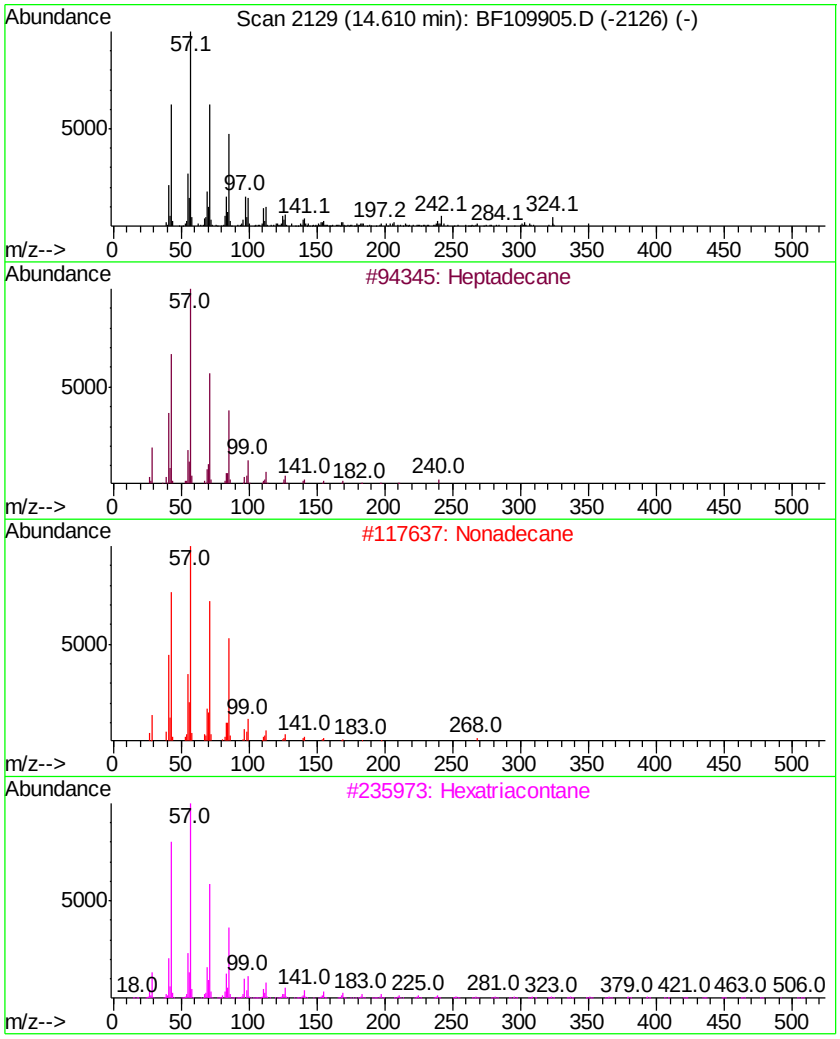
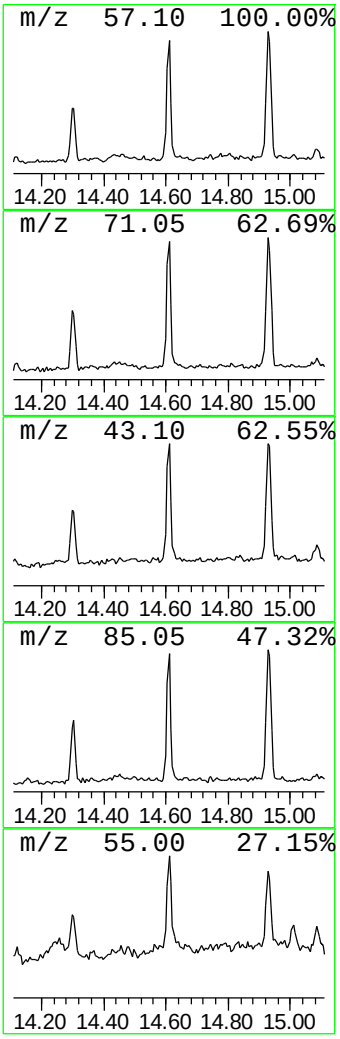
Peak Number 9 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	2.42 ng	248734	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	96
2	Nonadecane	268	C19H40	000629-92-5	90
3	Hexatriacontane	507	C36H74	000630-06-8	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Hentriacontane	437	C31H64	000630-04-6	87





Library Search Compound Report

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Acq On : 16 Oct 2018 15:13
Operator : JU/SJ
Sample : J5526-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-4B-C-101518-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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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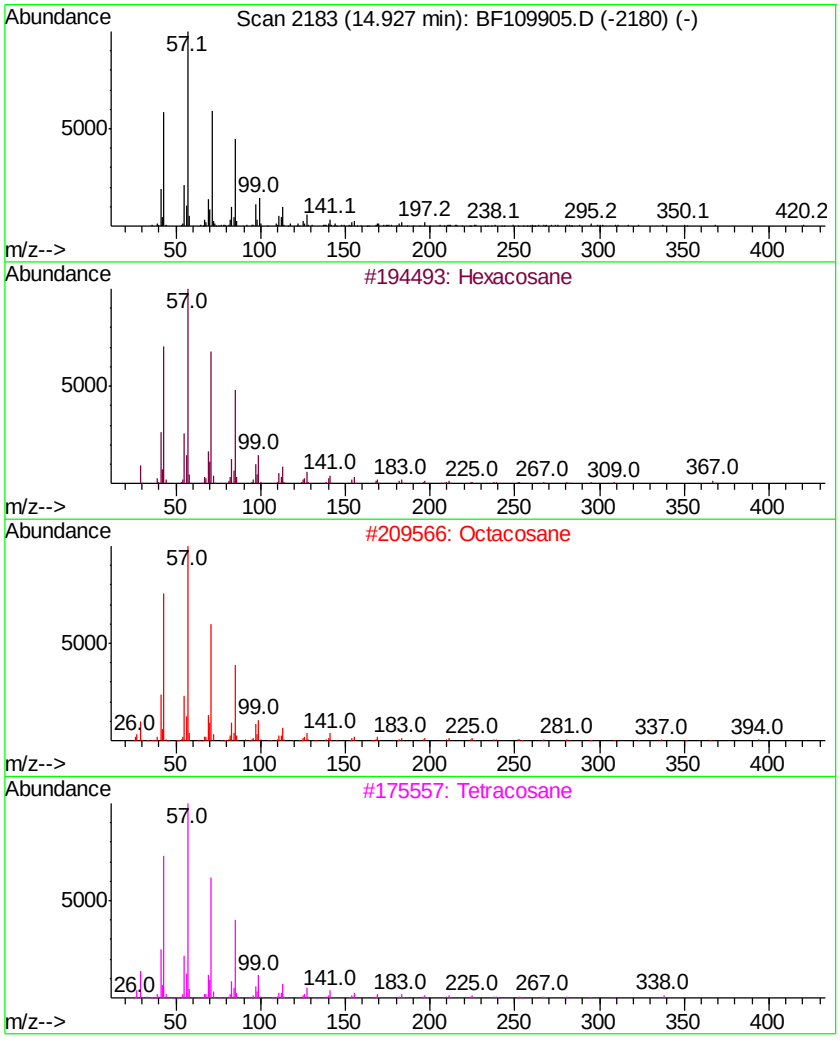
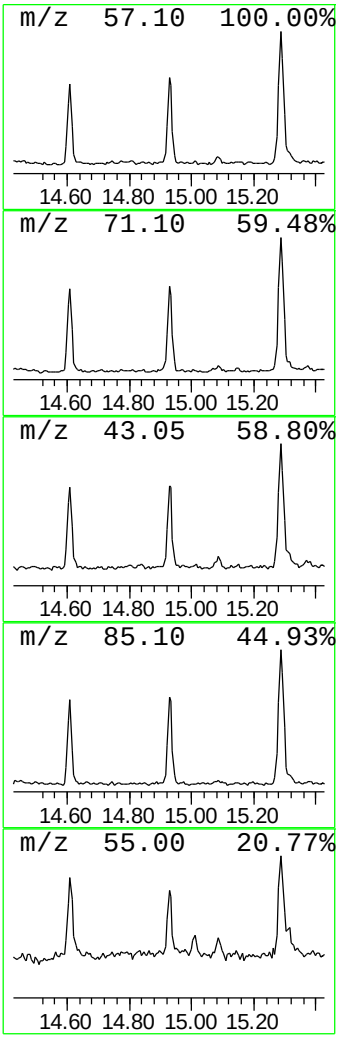
Peak Number 10 Hexacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	2.21 ng	253364	Perylene-d12	15.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Octacosane	394	C28H58	000630-02-4	90
3	Tetracosane	338	C24H50	000646-31-1	87
4	Heptacosane	380	C27H56	000593-49-7	87
5	Tridecane, 7-hexyl-	268	C19H40	007225-66-3	87





Library Search Compound Report

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Data File : BF109905.D
Acq On : 16 Oct 2018 15:13
Operator : JU/SJ
Sample : J5526-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-4B-C-101518-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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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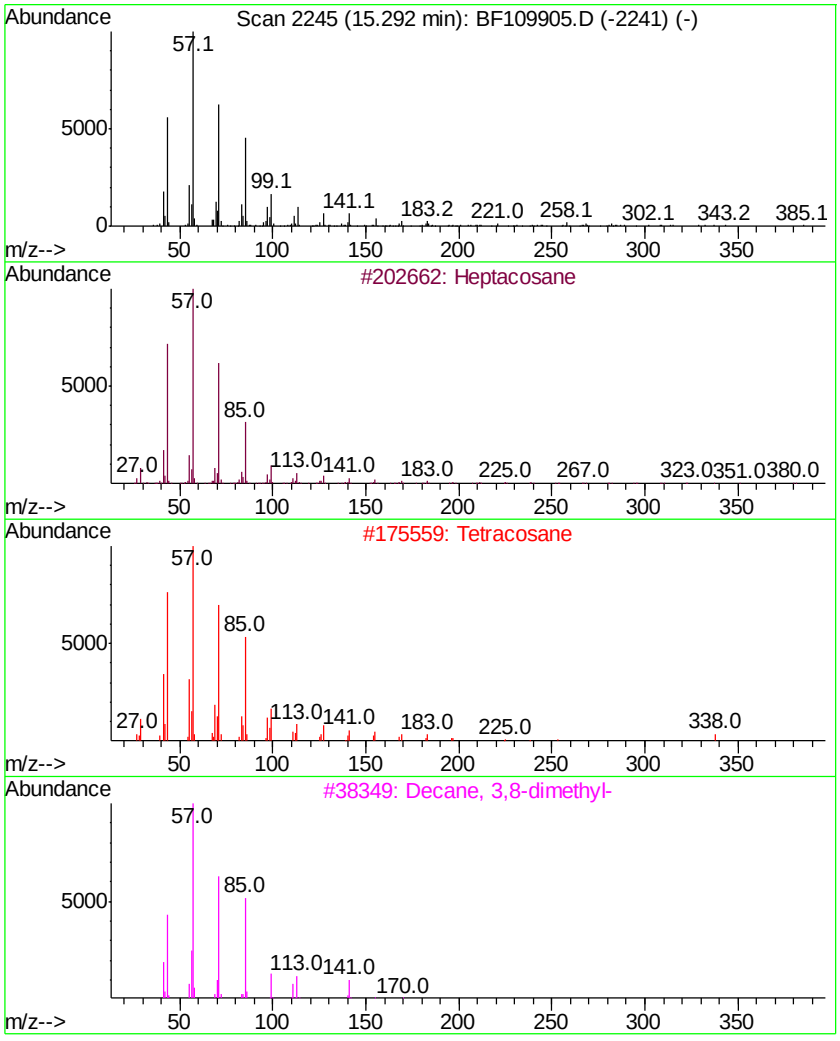
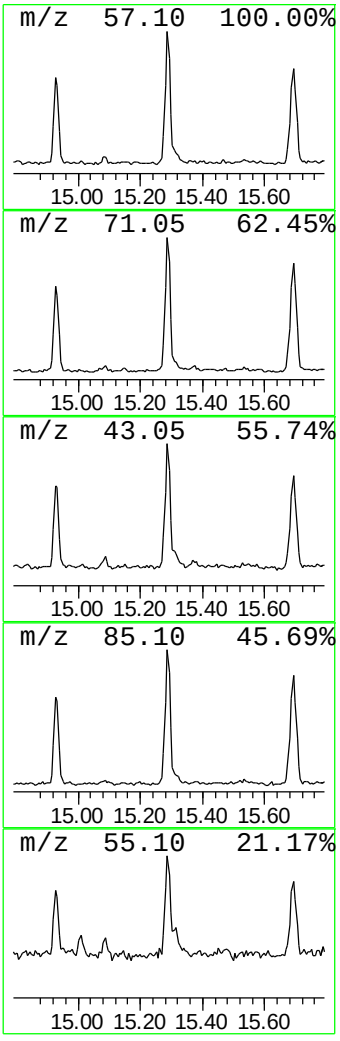
Peak Number 11 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.29	3.56 ng	408498	Perylene-d12	15.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	90
4	Octadecane	254	C18H38	000593-45-3	87
5	Heptadecane	240	C17H36	000629-78-7	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101618\
Data File : BF109905.D
Acq On : 16 Oct 2018 15:13
Operator : JU/SJ
Sample : J5526-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-4B-C-101518-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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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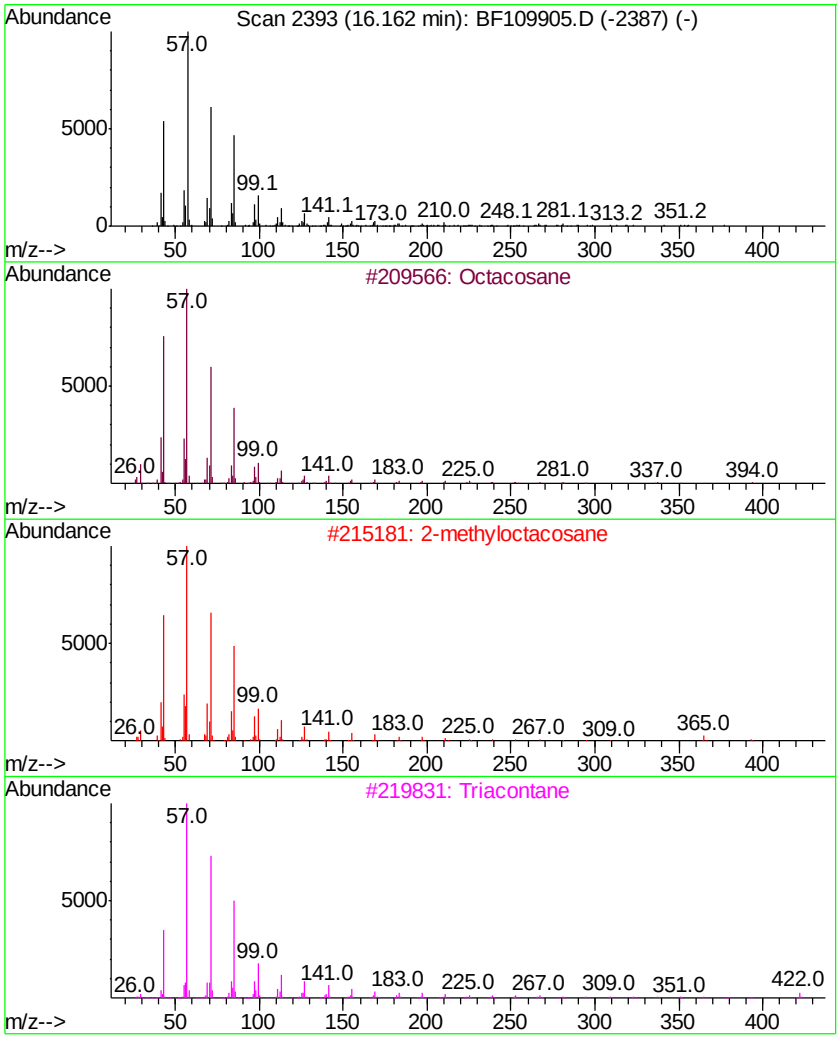
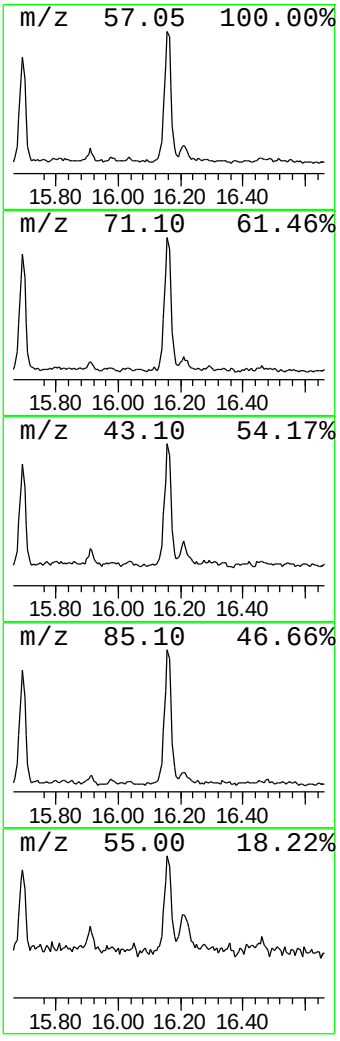
Peak Number 12 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.16	4.32 ng	495168	Perylene-d12	15.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	87
2	2-methyloctacosane	408	C29H60	1000376-72-8	87
3	Triacontane	422	C30H62	000638-68-6	87
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	86
5	Octadecane	254	C18H38	000593-45-3	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101618\
Data File : BF109905.D
Acq On : 16 Oct 2018 15:13
Operator : JU/SJ
Sample : J5526-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-4B-C-101518-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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...	2.32	11.9	ng	942955	1	6.98	1590730	20.0
2-Pentanone, 4-hy...	5.22	2.4	ng	187458	1	6.98	1590730	20.0
unknown6.75	6.75	57.6	ng	4582840	1	6.98	1590730	20.0
n-Hexadecanoic acid	12.02	2.8	ng	195501	4	11.51	1411650	20.0
n-Heptadecanol-1	12.54	2.1	ng	146658	4	11.51	1411650	20.0
Octadecanoic acid	12.80	2.6	ng	183095	4	11.51	1411650	20.0
Cyclopentadecane	13.97	7.0	ng	722304	5	14.16	2058570	20.0
Heptadecane	14.61	2.4	ng	248734	5	14.16	2058570	20.0
Hexacosane	14.93	2.2	ng	253364	6	15.69	2293390	20.0
Heptacosane	15.29	3.6	ng	408498	6	15.69	2293390	20.0
Octacosane	16.16	4.3	ng	495168	6	15.69	2293390	20.0