LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121218\
Data File : BF111332.D
Acq On : 12 Dec 2018 20:11
Operator : JU/SJ
Sample : J6214-21
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-8(0-2)

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-BF121218.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	3.234	193	195	201	rBV	40798	78563	1.14%	0.129%
2	5.004	492	496	502	rVB	295082	374457	5.45%	0.616%
3	5.416	561	566	569	rBV	5758650	6010824	87.51%	9.891%
4	6.428	733	738	749	rBV	6162959	6869079	100.00%	11.303%
5	6.563	756	761	764	rBV	6662911	6346961	92.40%	10.444%
6	6.792	796	800	803	rBV	2073615	1616352	23.53%	2.660%
7	6.951	823	827	830	rBV	5953082	4958346	72.18%	8.159%
8	7.351	889	895	898	rBV	4387422	4169671	60.70%	6.861%
9	8.075	1014	1018	1021	rBV	2528103	2082261	30.31%	3.426%
10	8.786	1134	1139	1144	rVB	73019	68741	1.00%	0.113%
11	9.151	1196	1201	1204	rBV	6957476	6045473	88.01%	9.948%
12	9.539	1264	1267	1276	rVB	775034	701870	10.22%	1.155%
13	9.686	1289	1292	1296	rVB	152635	121439	1.77%	0.200%
14	9.828	1311	1316	1320	rBV2	2234583	1912316	27.84%	3.147%
15	10.033	1347	1351	1355	rVB	86802	78404	1.14%	0.129%
16	10.239	1382	1386	1389	rBV2	61058	77186	1.12%	0.127%
17	10.610	1445	1449	1453	rBV	2717056	2639921	38.43%	4.344%
18	10.739	1468	1471	1478	rVB3	78600	106587	1.55%	0.175%
19	11.310	1564	1568	1570	rBV	1827273	1473770	21.46%	2.425%
20	11.333	1570	1572	1576	rVV	690682	539220	7.85%	0.887%
21	11.386	1578	1581	1583	rVB	147668	137864	2.01%	0.227%
22	11.810	1651	1653	1655	rBV	110325	92658	1.35%	0.152%
23	11.845	1655	1659	1663	rVV2	1204859	1172426	17.07%	1.929%
24	11.880	1663	1665	1669	rVV2	146406	186840	2.72%	0.307%
25	11.922	1669	1672	1674	rVV	213340	230378	3.35%	0.379%
26	11.945	1674	1676	1679	rVB	98321	91835	1.34%	0.151%
27	12.110	1701	1704	1705	rBV	89749	89143	1.30%	0.147%
28	12.363	1744	1747	1750	rBV	119675	128791	1.87%	0.212%
29	12.445	1758	1761	1766	rBV4	75021	100231	1.46%	0.165%
30	12.522	1770	1774	1777	rBV	1419186	1213347	17.66%	1.997%
31	12.633	1789	1793	1798	rBV2	758151	813543	11.84%	1.339%
32	12.751	1807	1813	1816	rBV	1112861	1158320	16.86%	1.906%
33	12.898	1834	1838	1841	rBV	4125976	3616897	52.65%	5.952%
34	13.080	1867	1869	1872	rVB	181622	141387	2.06%	0.233%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121218\
Data File : BF111332.D
Acq On : 12 Dec 2018 20:11
Operator : JU/SJ
Sample : J6214-21
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-8(0-2)

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-BF121218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.139	1877	1879	1882	rVB2	166554	168771	2.46%	0.278%
36	13.480	1935	1937	1939	rBV	167830	139401	2.03%	0.229%
37	13.810	1990	1993	1997	rVB	431662	396826	5.78%	0.653%
38	13.945	2012	2016	2019	rBV2	1701210	2236693	32.56%	3.680%
39	13.974	2019	2021	2026	rVB	595747	538380	7.84%	0.886%
40	14.127	2045	2047	2050	rBV2	213472	169490	2.47%	0.279%
41	14.974	2188	2191	2193	rBV	399859	500165	7.28%	0.823%
42	15.321	2248	2250	2255	rVB	331392	309240	4.50%	0.509%
43	15.386	2257	2261	2264	rBV	712546	867917	12.64%	1.428%

Sum of corrected areas: 60771984

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121218\
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Acq On : 12 Dec 2018 20:11
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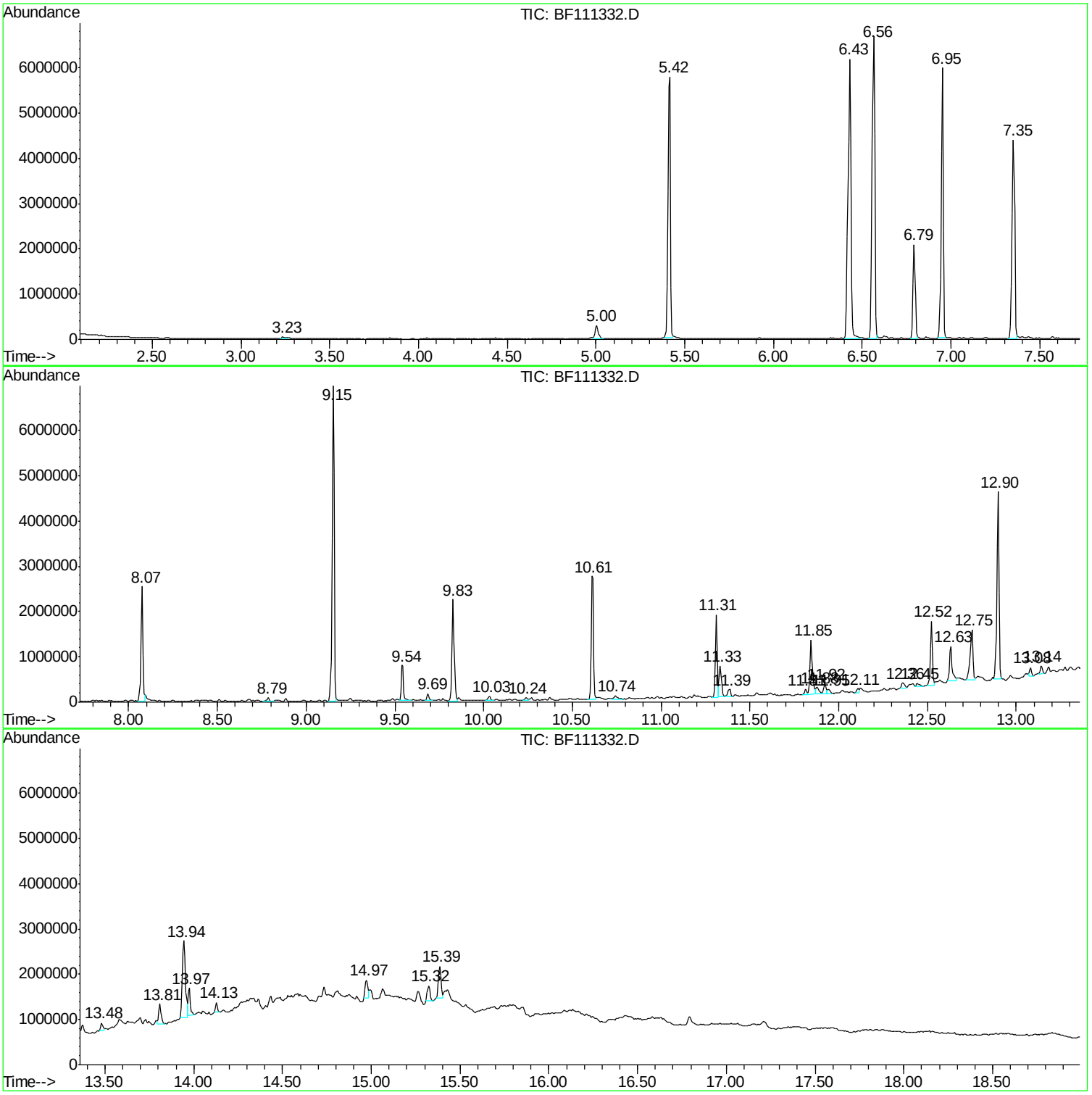
Sample : J6214-21
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-8(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.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\BF121218\
Data File : BF111332.D
Acq On : 12 Dec 2018 20:11
Operator : JU/SJ
Sample : J6214-21
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-8(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

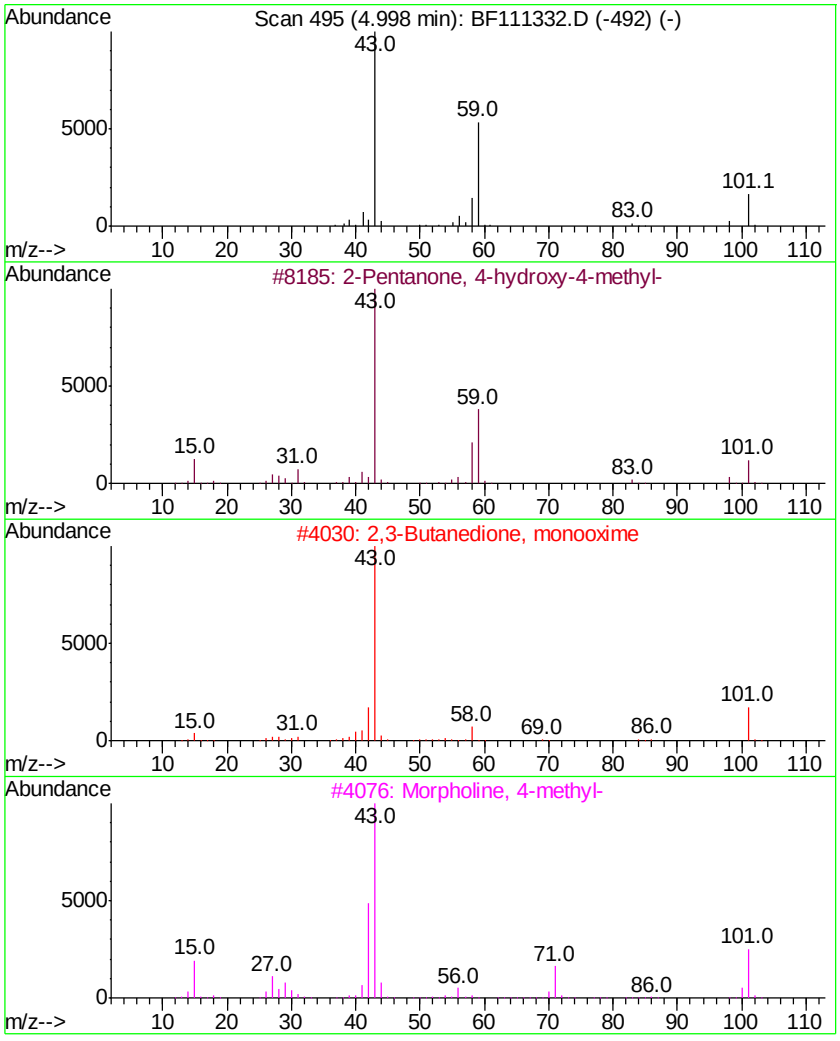
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

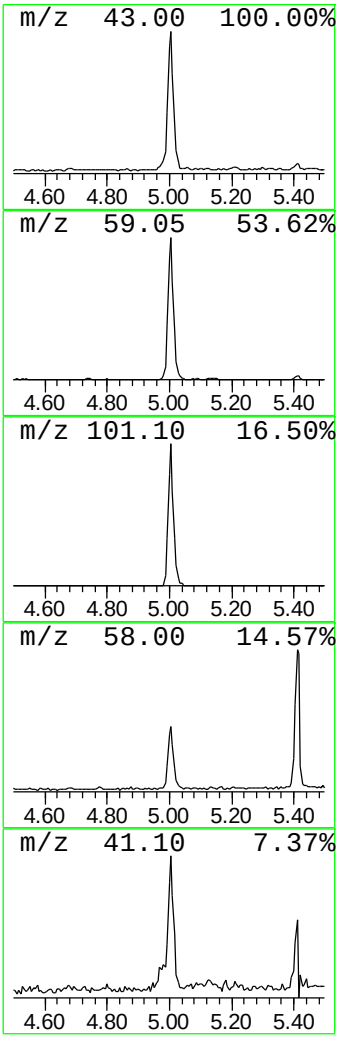
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	4.63 ng	374457	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	3-Octanol	130	C8H18O	000589-98-0	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121218\
Data File : BF111332.D
Acq On : 12 Dec 2018 20:11
Operator : JU/SJ
Sample : J6214-21
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-8(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

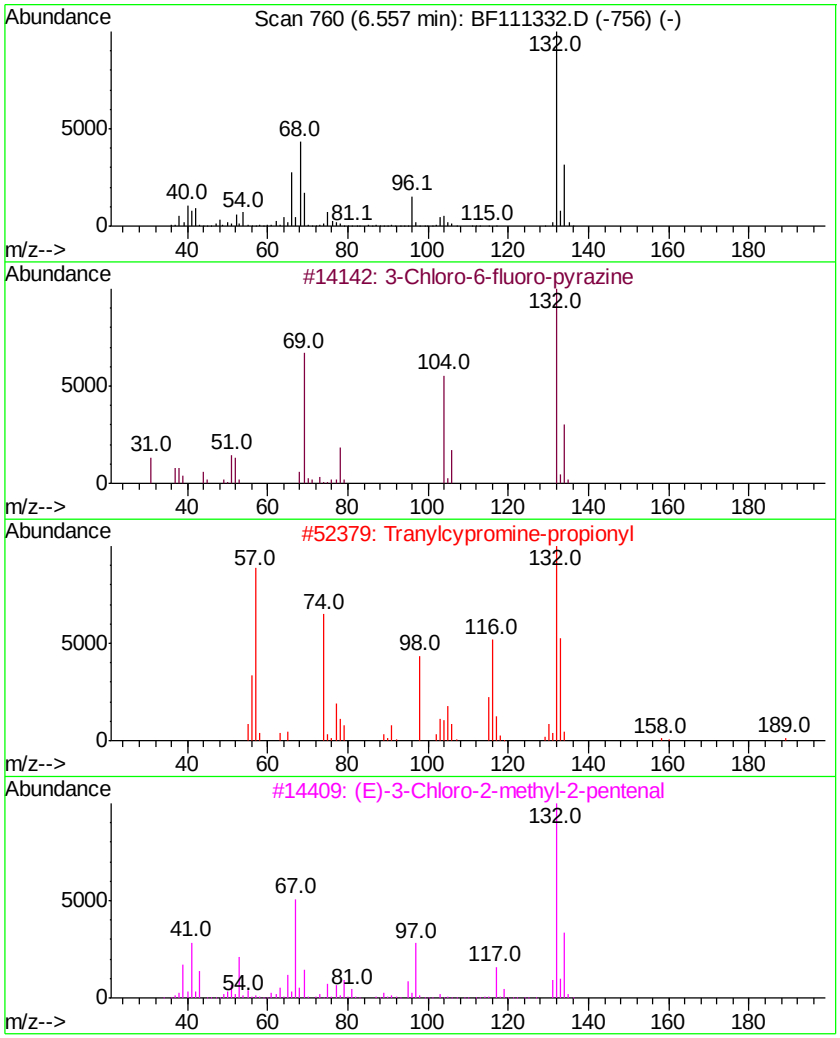
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

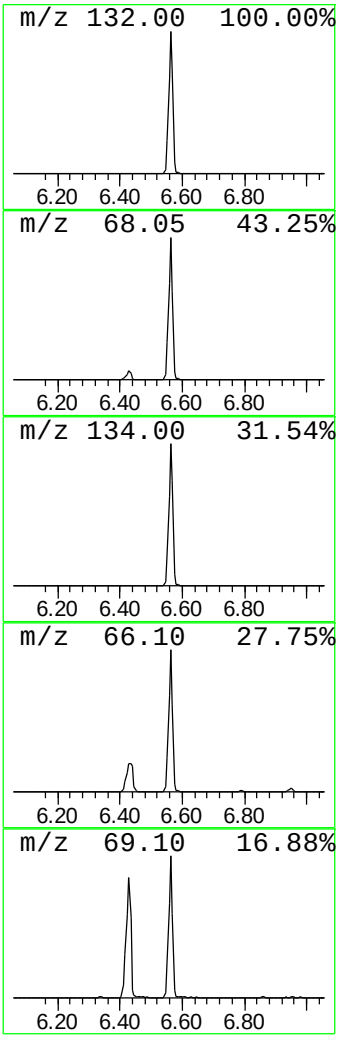
****

Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	78.53 ng	6346960	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4	Amphetaminil	250	C17H18N2	017590-01-1	12
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121218\
Data File : BF111332.D
Acq On : 12 Dec 2018 20:11
Operator : JU/SJ
Sample : J6214-21
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-8(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.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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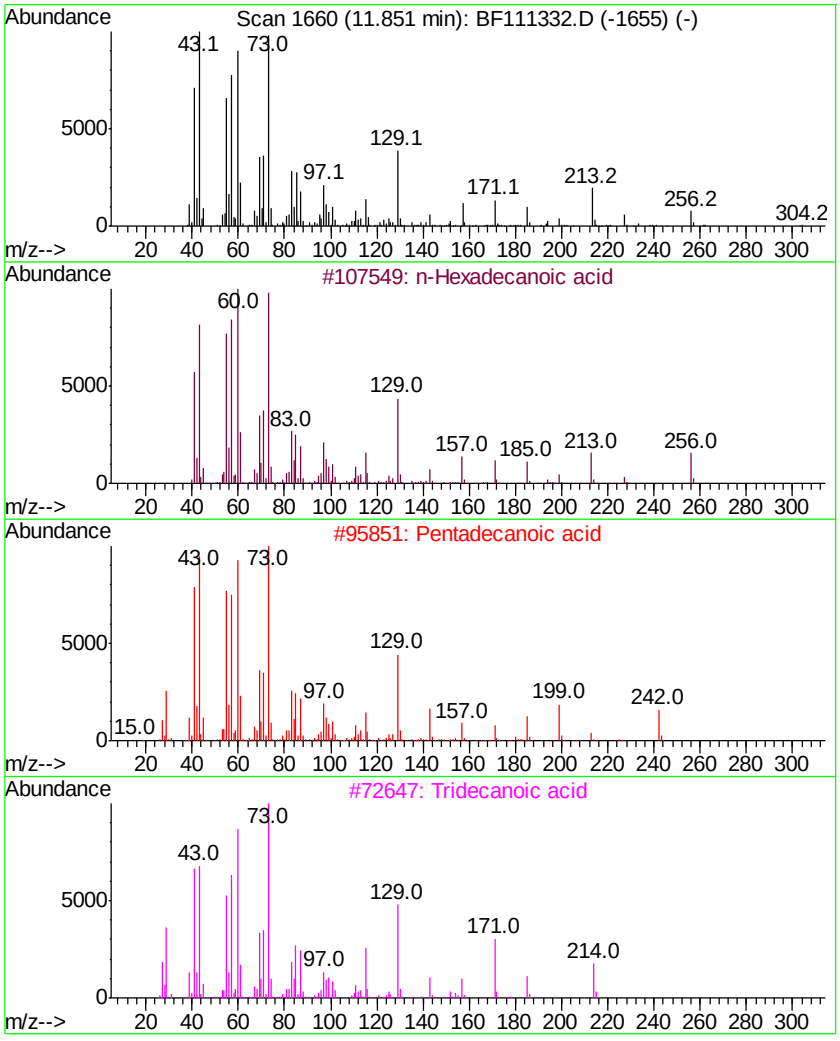
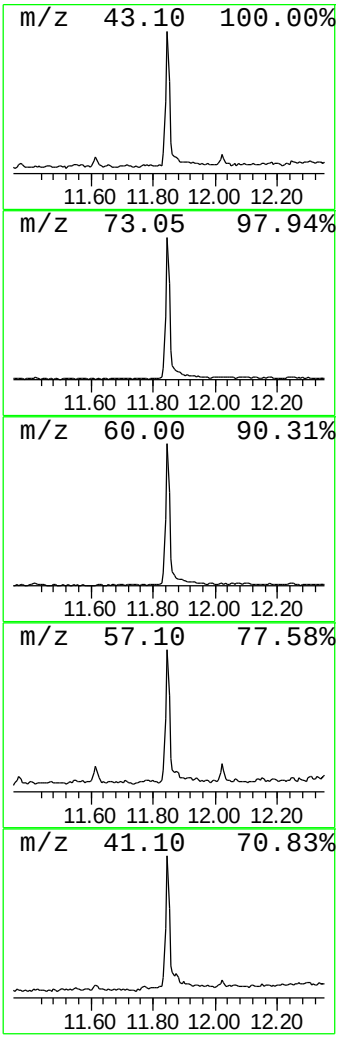
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	15.91 ng	1172430	Phenanthrene-d10	11.31

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	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	70
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	70
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121218\
Data File : BF111332.D
Acq On : 12 Dec 2018 20:11
Operator : JU/SJ
Sample : J6214-21
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-8(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.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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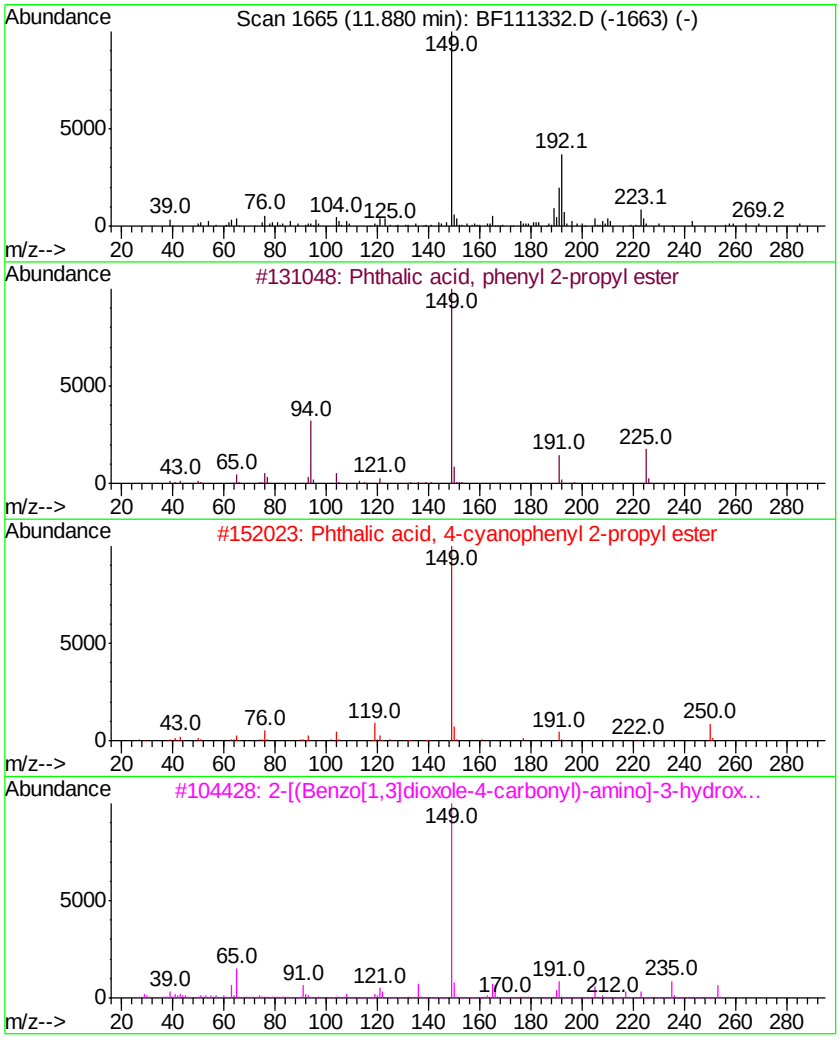
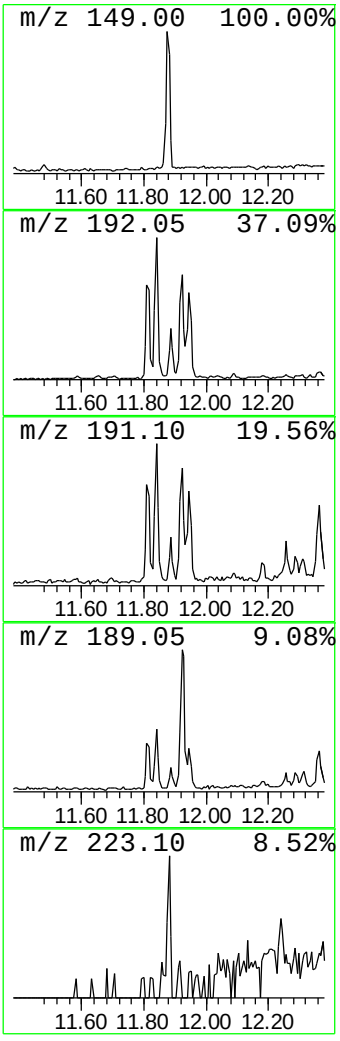
Peak Number 5 unknown11.88 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	2.54 ng	186840	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, phenyl 2-propyl e...	284	C17H16O4	1000315-56-5	47
2	Phthalic acid, 4-cyanophenyl 2-p...	309	C18H15NO4	1000315-57-1	43
3	2-[(Benzo[1,3]dioxole-4-carbonyl...	253	C11H11NO6	1000194-74-0	43
4	Dibutyl phthalate	278	C16H22O4	000084-74-2	43
5	Phthalic acid, butyl (2-chlorocy...	352	C19H25ClO4	1000315-34-3	43





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121218\
Data File : BF111332.D
Acq On : 12 Dec 2018 20:11
Operator : JU/SJ
Sample : J6214-21
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-8(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

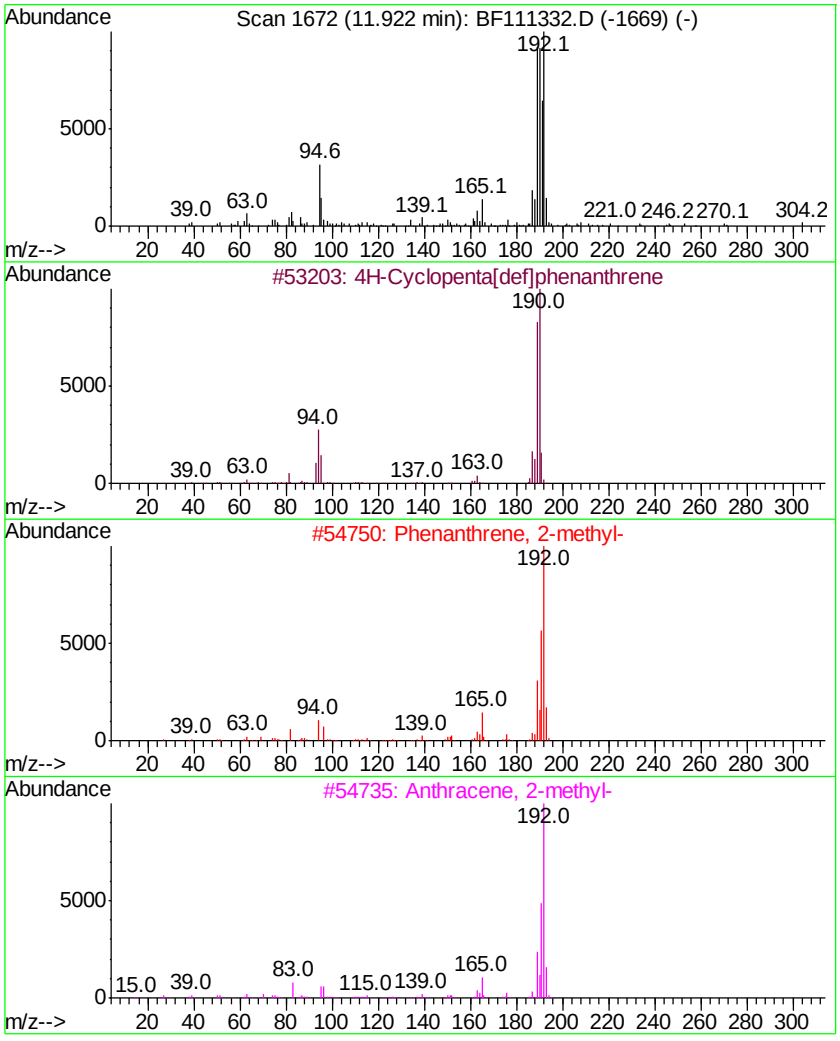
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

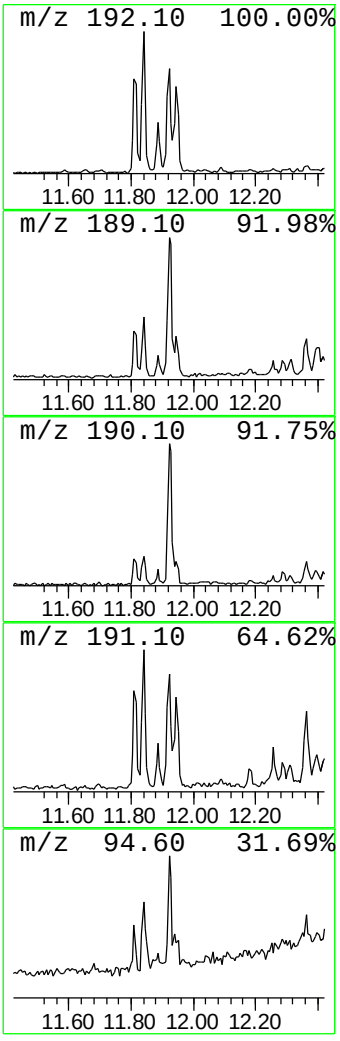
****

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	3.13 ng	230378	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	60
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	46
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	46
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	46
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	45





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121218\
Data File : BF111332.D
Acq On : 12 Dec 2018 20:11
Operator : JU/SJ
Sample : J6214-21
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-8(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

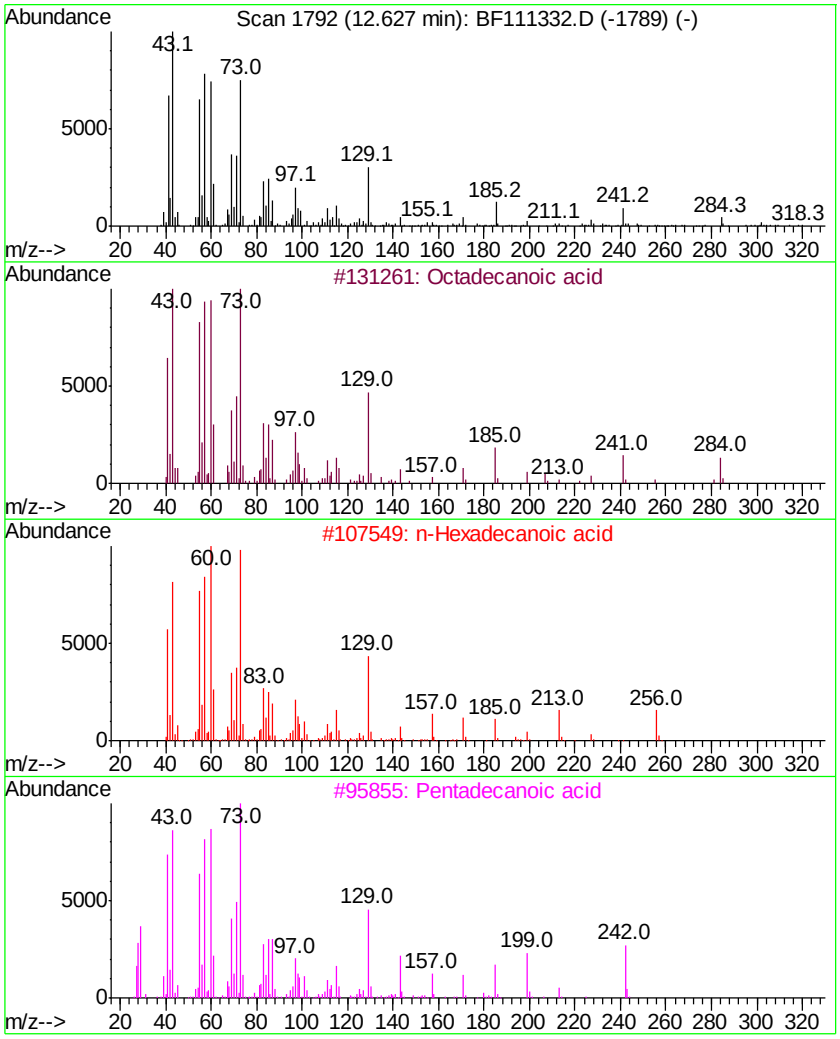
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

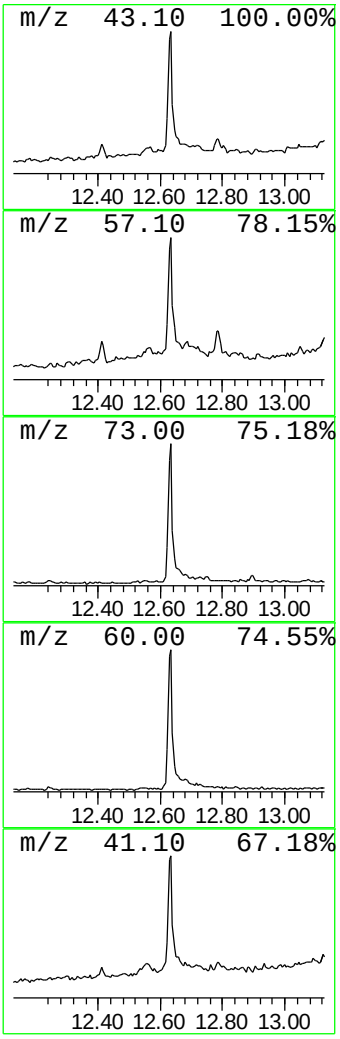
****

Peak Number 7 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	7.27 ng	813543	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5	Tridecanoic acid	214	C13H26O2	000638-53-9	62





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121218\
Data File : BF111332.D
Acq On : 12 Dec 2018 20:11
Operator : JU/SJ
Sample : J6214-21
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-8(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

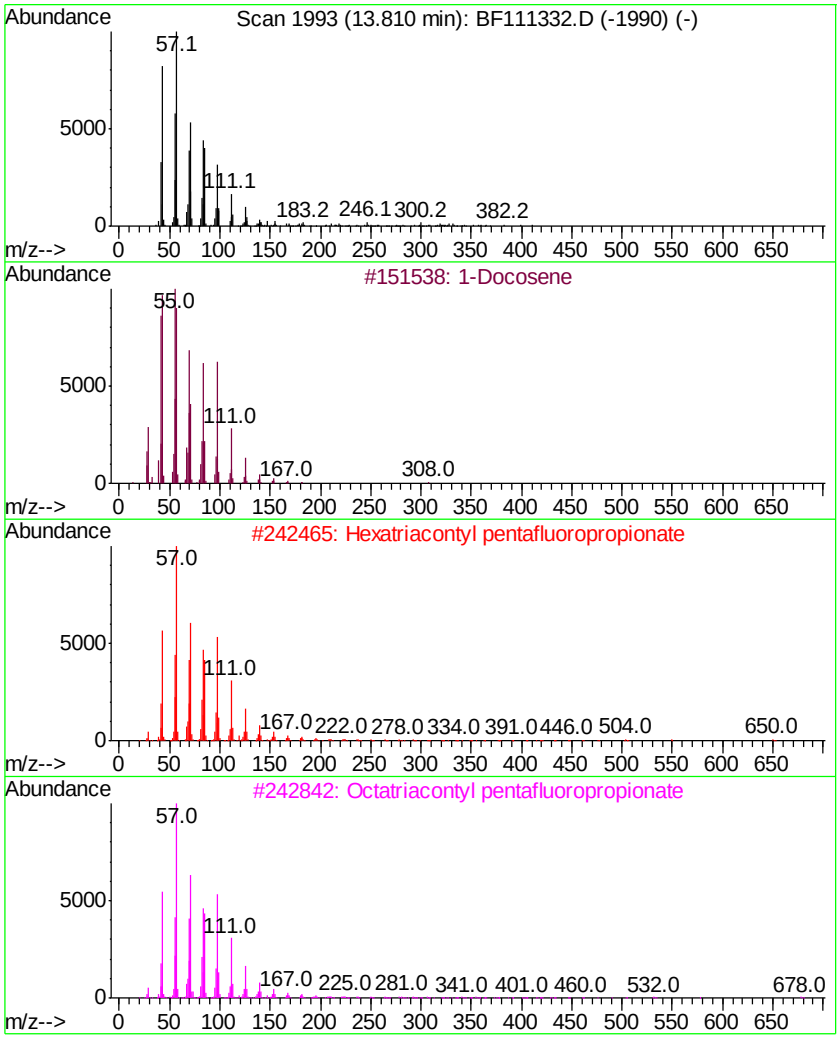
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

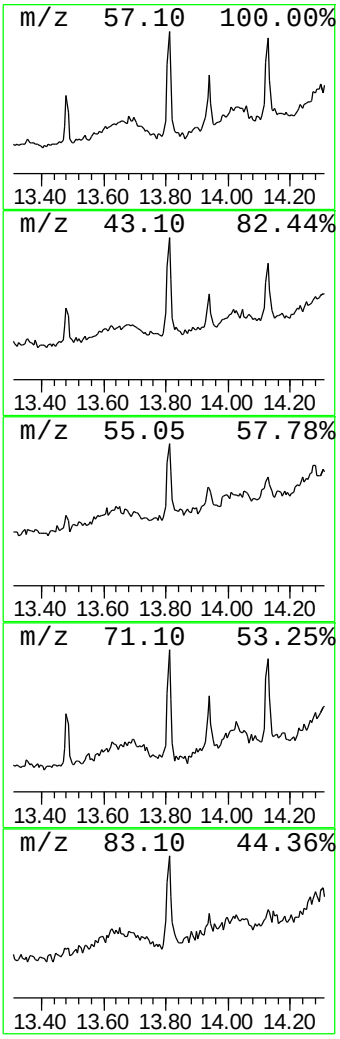
****

Peak Number 8 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	3.55 ng	396826	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	98
2	Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	91
3	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	91
4	Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1000351-81-4	87
5	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121218\
Data File : BF111332.D
Acq On : 12 Dec 2018 20:11
Operator : JU/SJ
Sample : J6214-21
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-8(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.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...	5.00	4.6	ng	374457	1	6.79	1616350	20.0
unknown6.56	6.56	78.5	ng	6346960	1	6.79	1616350	20.0
n-Hexadecanoic acid	11.85	15.9	ng	1172430	4	11.31	1473770	20.0
unknown11.88	11.88	2.5	ng	186840	4	11.31	1473770	20.0
4H-Cyclopenta[def...	11.92	3.1	ng	230378	4	11.31	1473770	20.0
Octadecanoic acid	12.63	7.3	ng	813543	5	13.95	2236690	20.0
1-Docosene	13.81	3.5	ng	396826	5	13.95	2236690	20.0