LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060217\
Data File : BF095643.D
Acq On : 2 Jun 2017 20:04
Operator : SJ/MA
Sample : I3412-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-TP-2-COMP

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-BF050217.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	4.787	523	527	543	rBV	54074	151385	7.30%	0.889%
2	5.451	636	640	670	rBV	823242	1781093	85.84%	10.459%
3	7.087	914	918	932	rBV	994570	1680038	80.97%	9.866%
4	7.192	932	936	964	rVB	1267572	2074891	100.00%	12.185%
5	7.539	991	995	1003	rBV	324090	449581	21.67%	2.640%
6	7.775	1030	1035	1050	rBV	1064036	1386282	66.81%	8.141%
7	8.451	1145	1150	1166	rBV	646541	1023716	49.34%	6.012%
8	9.569	1336	1340	1360	rBV	416270	611503	29.47%	3.591%
9	11.345	1636	1642	1655	rBV	1403793	1778847	85.73%	10.446%
10	12.039	1756	1760	1770	rVB	101582	136003	6.55%	0.799%
11	12.174	1780	1783	1789	rBV	17154	23412	1.13%	0.137%
12	12.392	1815	1820	1827	rBV2	463438	588010	28.34%	3.453%
13	12.445	1827	1829	1838	rVB2	16234	26044	1.26%	0.153%
14	13.239	1958	1964	1971	rBV3	17527	26710	1.29%	0.157%
15	13.304	1971	1975	1982	rVB2	15286	21940	1.06%	0.129%
16	13.692	2036	2041	2054	rBV	544611	817605	39.40%	4.801%
17	14.010	2090	2095	2098	rBV	23840	29983	1.45%	0.176%
18	14.739	2216	2219	2224	rBV3	18057	23060	1.11%	0.135%
19	14.798	2224	2229	2233	rVV2	351321	482796	23.27%	2.835%
20	14.833	2233	2235	2242	rVB	52118	77576	3.74%	0.456%
21	14.939	2249	2253	2262	rVB	19267	29653	1.43%	0.174%
22	15.598	2361	2365	2369	rBV	23055	26160	1.26%	0.154%
23	15.639	2369	2372	2377	rVV	22892	26460	1.28%	0.155%
24	15.745	2387	2390	2393	rBV2	28567	34322	1.65%	0.202%
25	15.786	2393	2397	2407	rVB2	63496	96486	4.65%	0.567%
26	16.398	2497	2501	2505	rBV	30716	34907	1.68%	0.205%
27	16.604	2532	2536	2541	rBV	122424	157903	7.61%	0.927%
28	16.874	2580	2582	2584	rVV3	38093	41216	1.99%	0.242%
29	16.904	2584	2587	2594	rVB	164483	202468	9.76%	1.189%
30	17.145	2623	2628	2636	rVB	1059464	1226159	59.10%	7.200%
31	17.227	2636	2642	2648	rBV5	16651	29733	1.43%	0.175%
32	17.345	2657	2662	2664	rBV4	17894	29496	1.42%	0.173%
33	17.374	2664	2667	2671	rVB	29908	35992	1.73%	0.211%
34	17.462	2679	2682	2686	rVB	21201	24403	1.18%	0.143%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060217\
Data File : BF095643.D
Acq On : 2 Jun 2017 20:04
Operator : SJ/MA
Sample : I3412-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-TP-2-COMP

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-BF050217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.504	2686	2689	2693	rBV2	30478	43768	2.11%	0.257%
36	17.621	2705	2709	2712	rBV2	25397	29228	1.41%	0.172%
37	17.662	2713	2716	2721	rVB	18261	21438	1.03%	0.126%
38	18.174	2798	2803	2805	rBV5	13250	23910	1.15%	0.140%
39	18.386	2835	2839	2850	rBV9	49600	108094	5.21%	0.635%
40	18.492	2852	2857	2862	rBV2	442760	608182	29.31%	3.571%
41	18.627	2875	2880	2883	rBV7	20577	30845	1.49%	0.181%
42	19.003	2939	2944	2949	rBV4	36971	61137	2.95%	0.359%
43	19.515	3027	3031	3042	rVB2	207605	300237	14.47%	1.763%
44	19.621	3047	3049	3055	rVB2	35324	42029	2.03%	0.247%
45	19.774	3071	3075	3078	rBV	69529	93196	4.49%	0.547%
46	20.062	3121	3124	3128	rBV	51215	58235	2.81%	0.342%
47	20.121	3131	3134	3139	rVV	57932	76861	3.70%	0.451%
48	20.168	3139	3142	3147	rBV	289405	345879	16.67%	2.031%

Sum of corrected areas: 17028872

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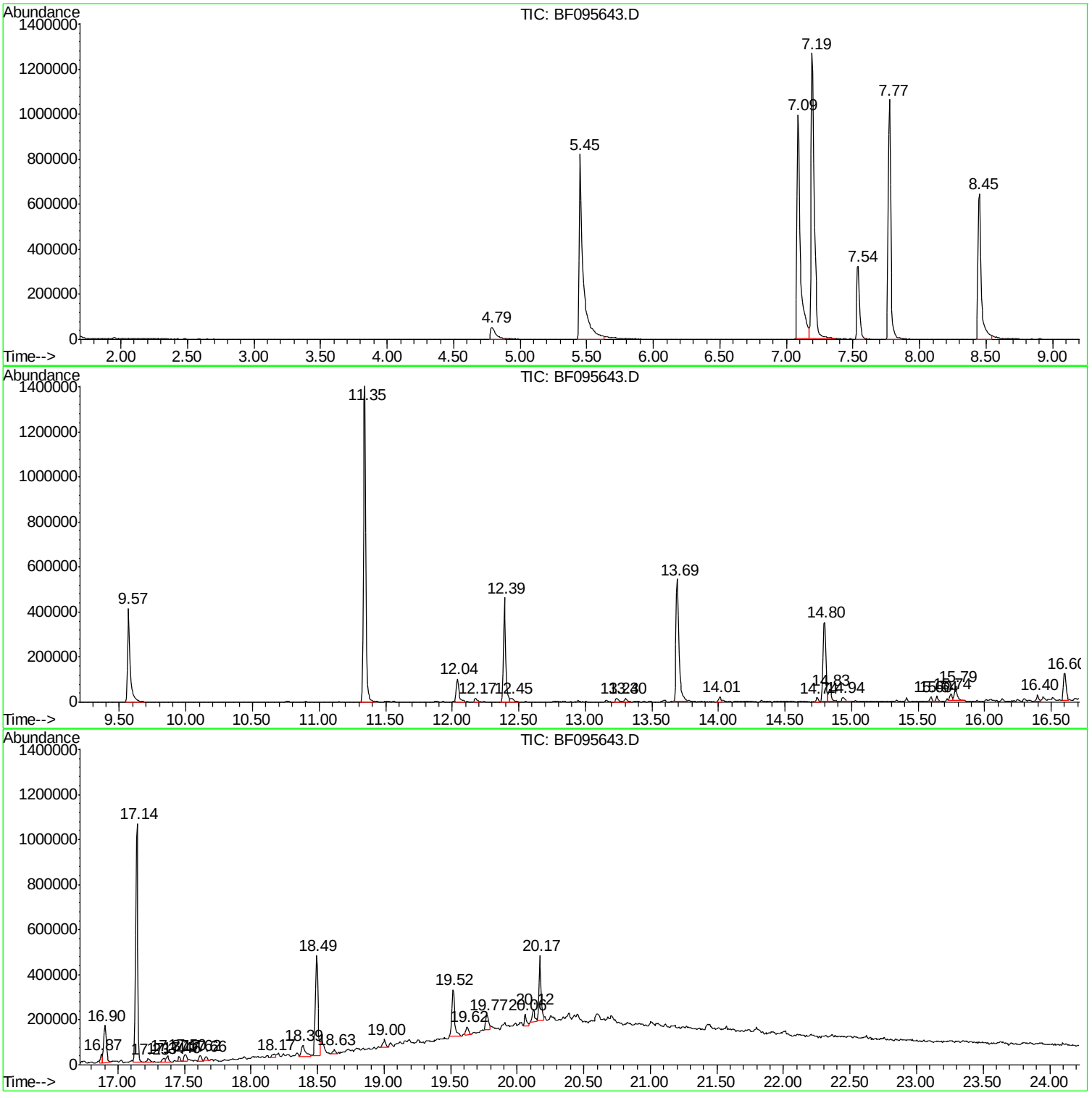
Instrument : BNA_F
ClientSampleId : TP-1-TP-2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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:\HPCHEM1\BNA F\DATA\BF060217\
Data File : BF095643.D
Acq On : 2 Jun 2017 20:04
Operator : SJ/MA
Sample : I3412-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-TP-2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

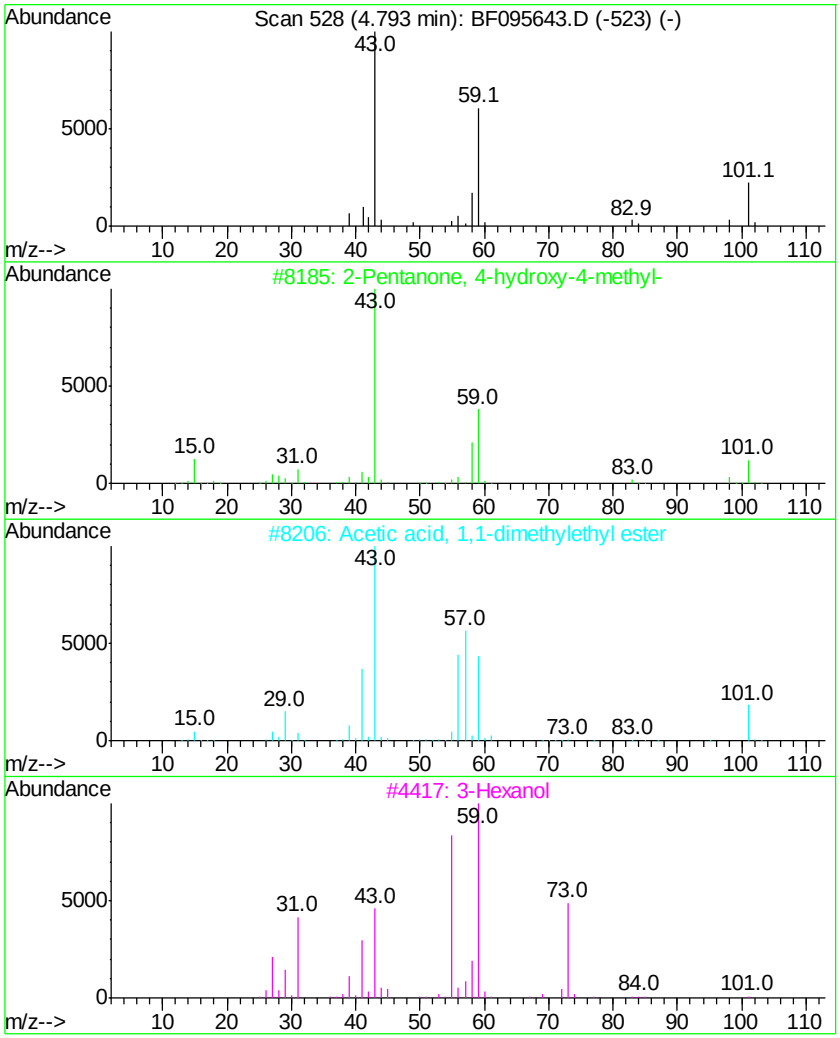
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

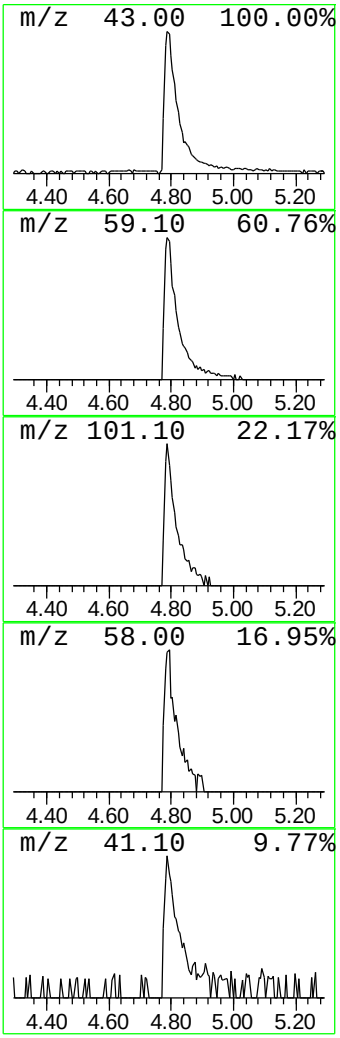
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	6.73 ng	151385	1,4-Dichlorobenzene-d4	7.54

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	50
3	3-Hexanol	102	C6H14O	000623-37-0	28
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060217\
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Operator : SJ/MA
Sample : I3412-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-TP-2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

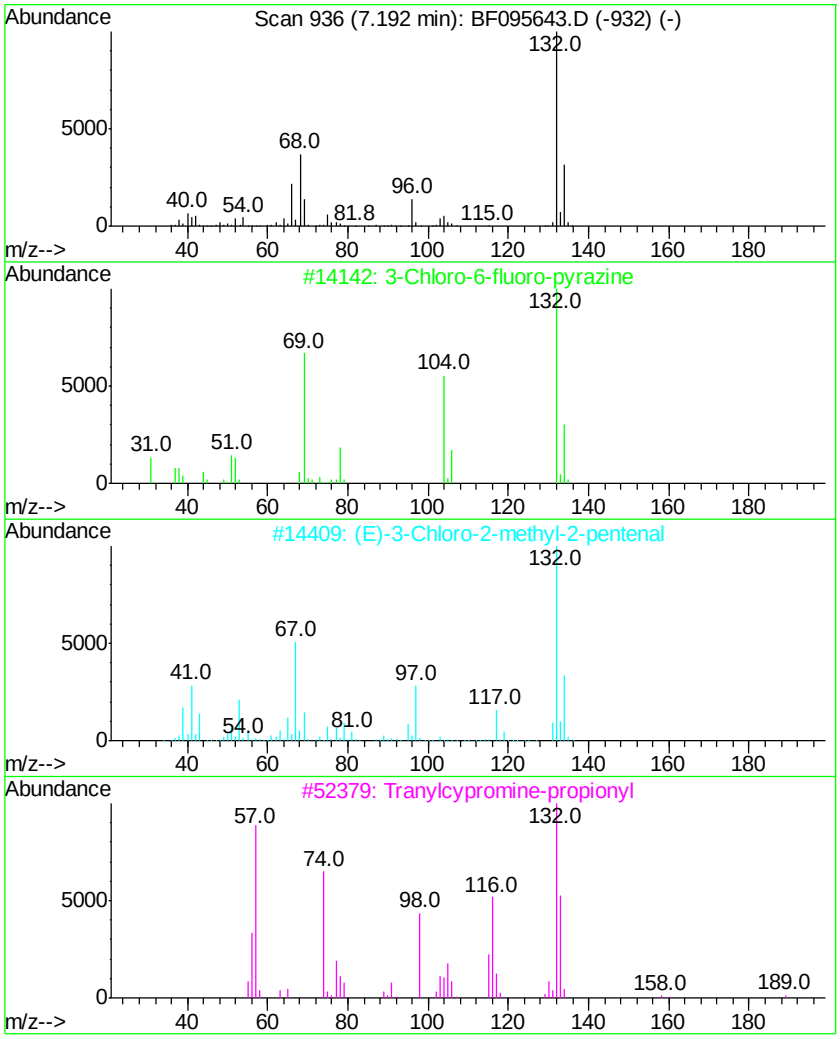
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

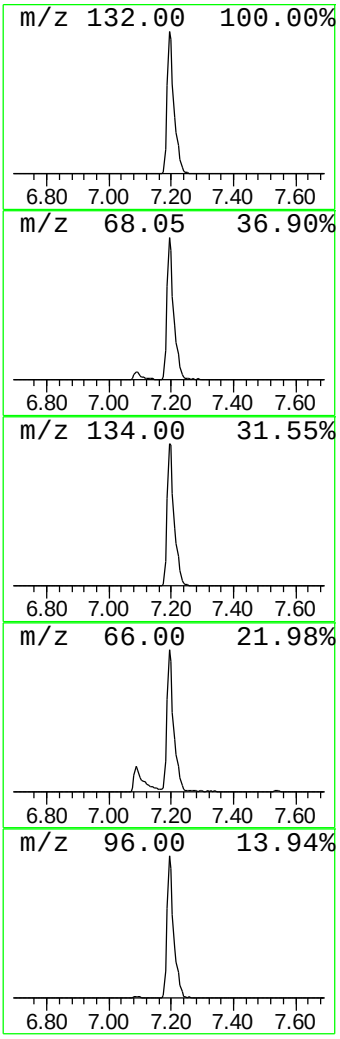
****

Peak Number 2 unknown7.19 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.19	92.30 ng	2074890	1,4-Dichlorobenzene-d4	7.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Xenon	132	Xe	007440-63-3	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Acq On : 2 Jun 2017 20:04
Operator : SJ/MA
Sample : I3412-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-TP-2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

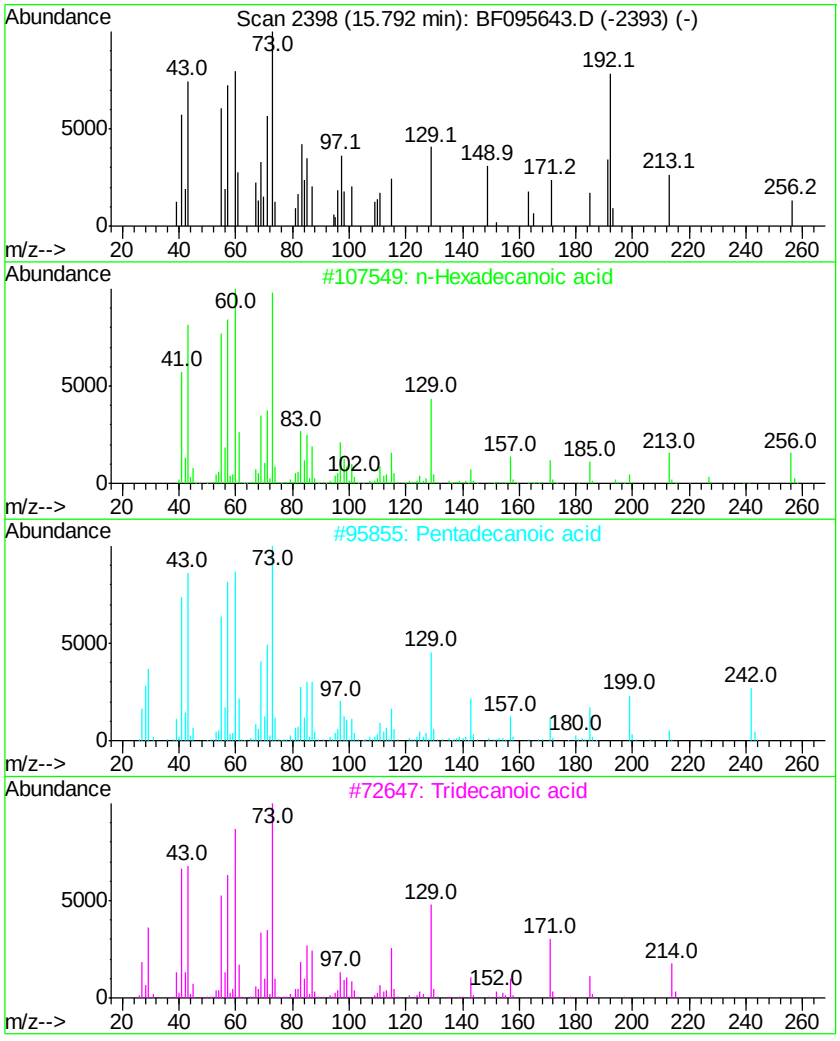
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

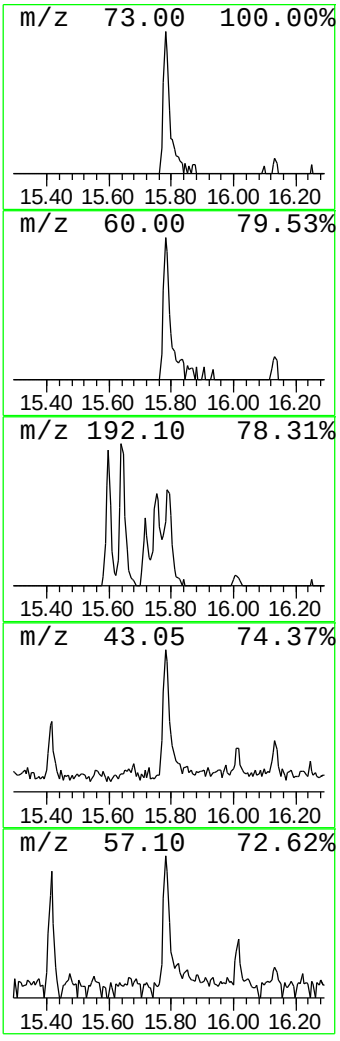
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	4.00 ng	96486	Phenanthrene-d10	14.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
3	Tridecanoic acid	214	C13H26O2	000638-53-9	62
4	n-Decanoic acid	172	C10H20O2	000334-48-5	50
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	50





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060217\
Data File : BF095643.D
Acq On : 2 Jun 2017 20:04
Operator : SJ/MA
Sample : I3412-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-TP-2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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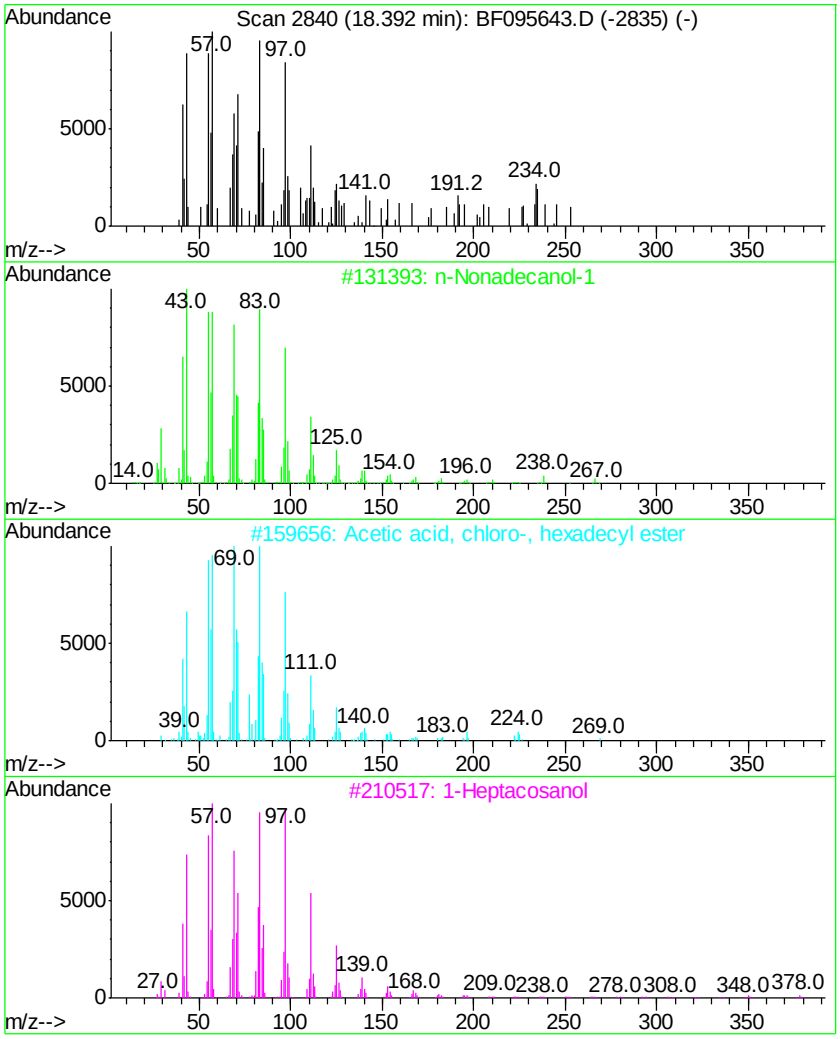
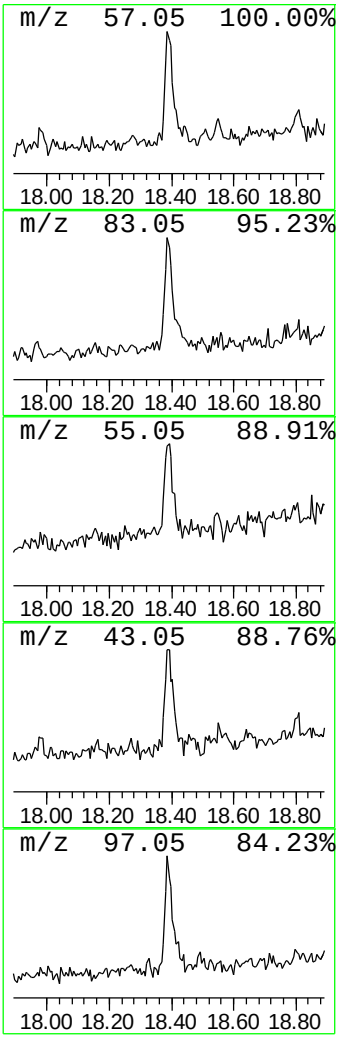
Peak Number 5 n-Nonadecanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.39	3.55 ng	108094	Chrysene-d12	18.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	87
2	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	86
3	1-Heptacosanol	396	C27H56O	002004-39-9	83
4	11-Tricosene	322	C23H46	052078-56-5	81
5	Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	68





Library Search Compound Report

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Acq On : 2 Jun 2017 20:04
Operator : SJ/MA
Sample : I3412-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-TP-2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

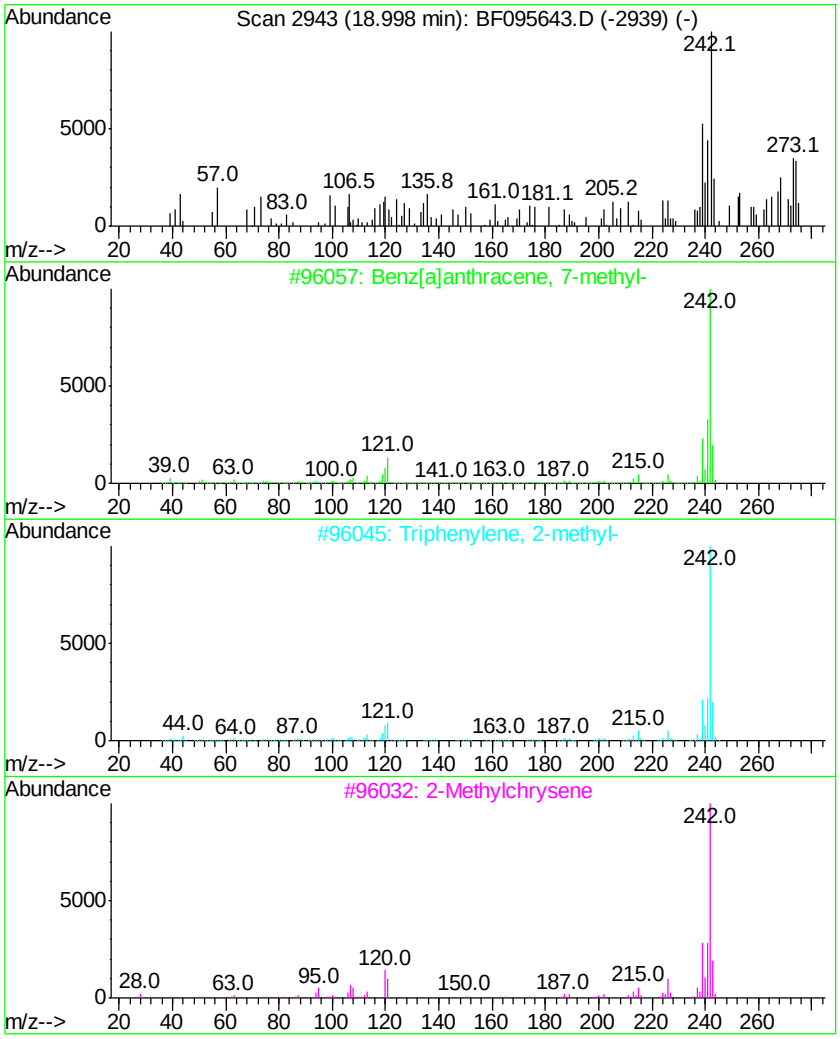
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

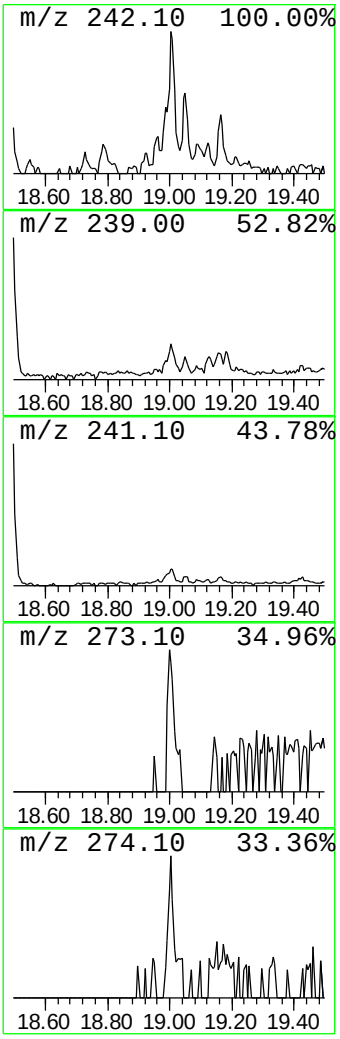
****

Peak Number 6 Benz[a]anthracene, 7-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.00	2.01 ng	61137	Chrysene-d12	18.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benz[a]anthracene, 7-methyl-	242	C19H14	002541-69-7	60
2	Triphenylene, 2-methyl-	242	C19H14	001705-84-6	49
3	2-Methylchrysene	242	C19H14	003351-32-4	49
4	Chrysene, 1-methyl-	242	C19H14	003351-28-8	49
5	Benz[a]anthracene, 8-methyl-	242	C19H14	002381-31-9	49





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Data File : BF095643.D
Acq On : 2 Jun 2017 20:04
Operator : SJ/MA
Sample : I3412-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-TP-2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

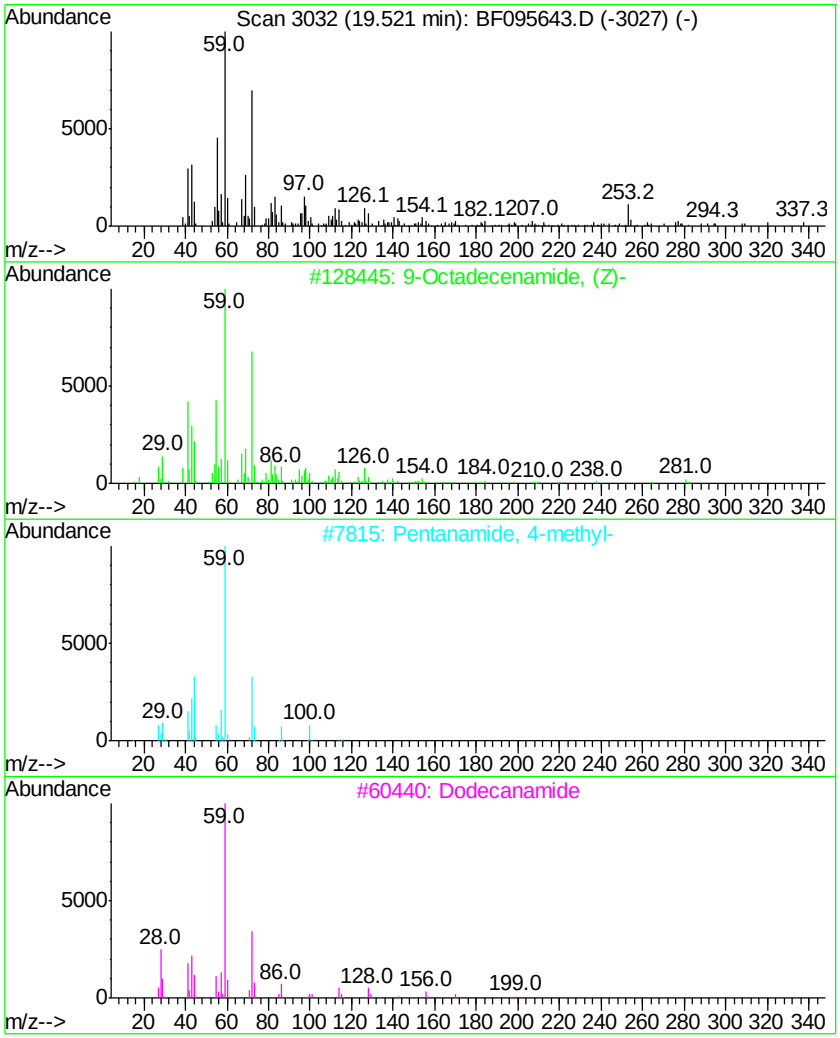
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

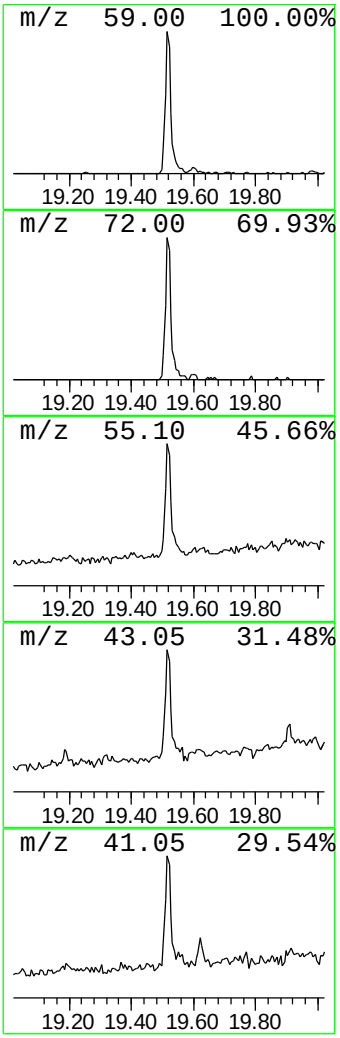
****

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.52	17.36 ng	300237	Perylene-d12	20.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	53
3	Dodecanamide	199	C12H25NO	001120-16-7	52
4	Decanamide-	171	C10H21NO	002319-29-1	50
5	2-Hydroxy-2,4-dimethyl-hept-6-en...	156	C9H16O2	1000192-56-0	38





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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-TP-2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

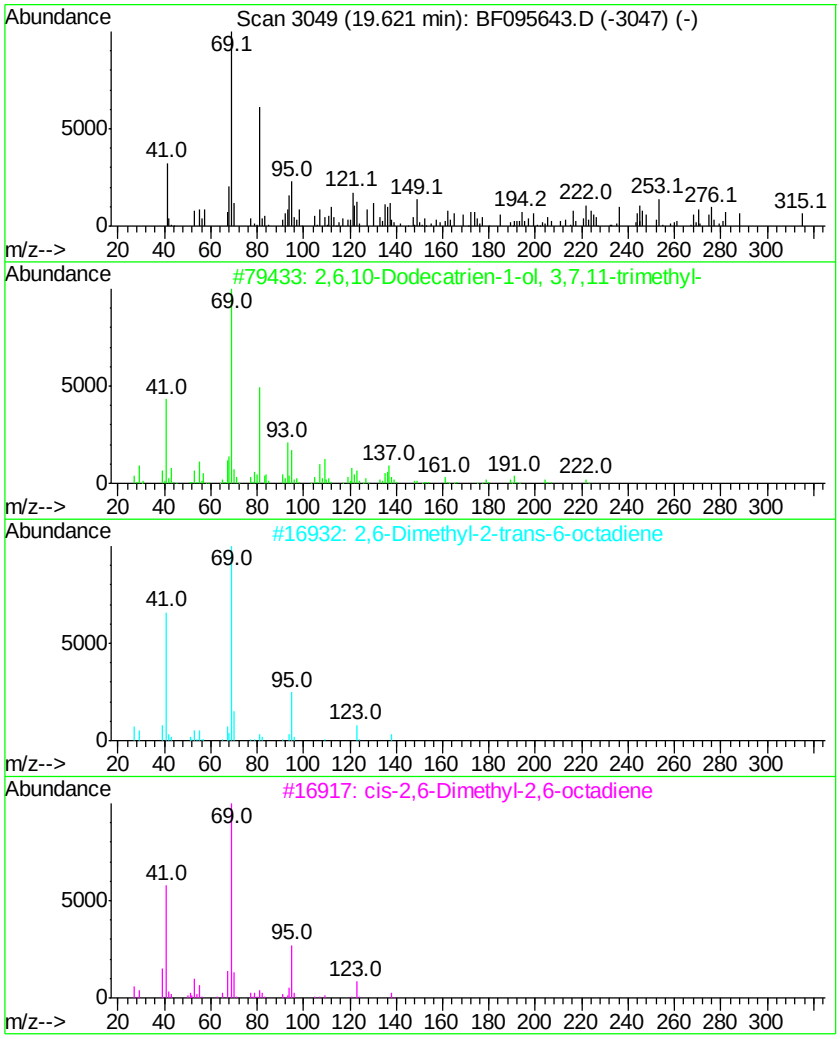
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

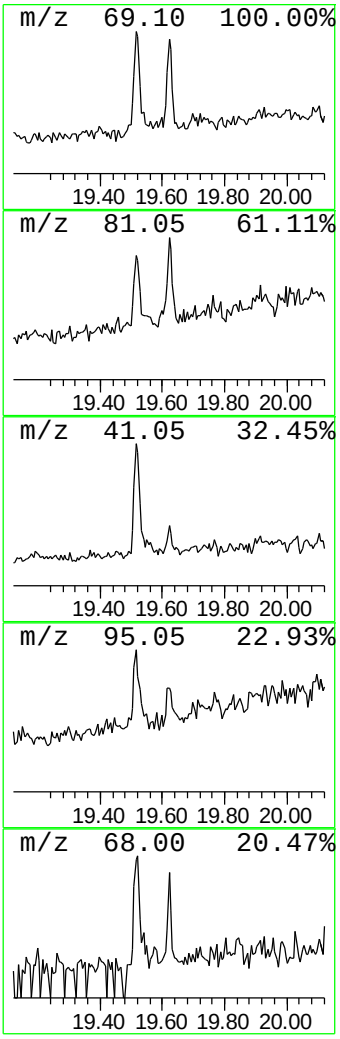
****

Peak Number 8 2,6,10-Dodecatrien-1-ol, 3,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.62	2.43 ng	42029	Perylene-d12	20.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	50
2	2,6-Dimethyl-2-trans-6-octadiene	138	C10H18	002609-23-6	49
3	cis-2,6-Dimethyl-2,6-octadiene	138	C10H18	002492-22-0	49
4	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	47
5	1,5-Heptadiene, 3,3,5-trimethyl-	138	C10H18	074630-29-8	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060217\
Data File : BF095643.D
Acq On : 2 Jun 2017 20:04
Operator : SJ/MA
Sample : I3412-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-TP-2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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...	4.79	6.7	ng	151385	1	7.54	449581	20.0
unknown7.19	7.19	92.3	ng	2074890	1	7.54	449581	20.0
n-Hexadecanoic acid	15.79	4.0	ng	96486	4	14.79	482796	20.0
n-Nonadecanol-1	18.39	3.5	ng	108094	5	18.49	608182	20.0
Benz[a]anthracene...	19.00	2.0	ng	61137	5	18.49	608182	20.0
9-Octadecenamide,...	19.52	17.4	ng	300237	6	20.17	345879	20.0
2,6,10-Dodecatrie...	19.62	2.4	ng	42029	6	20.17	345879	20.0