LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062618\
Data File : BG035438.D
Acq On : 27 Jun 2018 9:49
Operator : JU/SJ
Sample : J3687-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PE-1

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_G\METHODS\8270-BG060718.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	5.162	312	319	328	rVB	87346	141044	3.42%	0.620%
2	5.626	391	398	413	rVB	958463	1566203	38.00%	6.889%
3	7.212	660	668	683	rBV	1049396	1846702	44.81%	8.123%
4	7.588	724	732	740	rBV	951151	1680257	40.77%	7.391%
5	8.052	804	811	820	rVB	174100	301154	7.31%	1.325%
6	8.375	858	866	875	rBV	690055	1203005	29.19%	5.292%
7	9.209	999	1008	1018	rBV	607928	1083975	26.30%	4.768%
8	10.854	1280	1288	1296	rBV	238201	424832	10.31%	1.869%
9	13.298	1696	1704	1714	rBV	1630471	2539240	61.61%	11.170%
10	14.120	1838	1844	1854	rBV	190386	285610	6.93%	1.256%
11	14.673	1931	1938	1946	rBV2	403639	665980	16.16%	2.929%
12	16.159	2182	2191	2200	rBV	1526033	2422448	58.78%	10.656%
13	16.376	2223	2228	2238	rVB6	32308	61798	1.50%	0.272%
14	17.416	2398	2405	2412	rBV2	567967	885559	21.49%	3.895%
15	18.297	2551	2555	2564	rBV	250154	345533	8.38%	1.520%
16	19.560	2764	2770	2780	rBV	112060	172176	4.18%	0.757%
17	20.018	2842	2848	2857	rBV	3054921	4121463	100.00%	18.129%
18	21.322	3065	3070	3083	rBV2	119233	283767	6.89%	1.248%
19	21.681	3124	3131	3138	rBV	626578	1037075	25.16%	4.562%
20	22.527	3268	3275	3288	rBV8	55713	143573	3.48%	0.632%
21	24.894	3668	3678	3688	rBV2	329493	946997	22.98%	4.166%
22	25.910	3839	3851	3863	rVB3	157881	484329	11.75%	2.130%
23	27.496	4112	4121	4133	rBV3	27567	90894	2.21%	0.400%

Sum of corrected areas: 22733614

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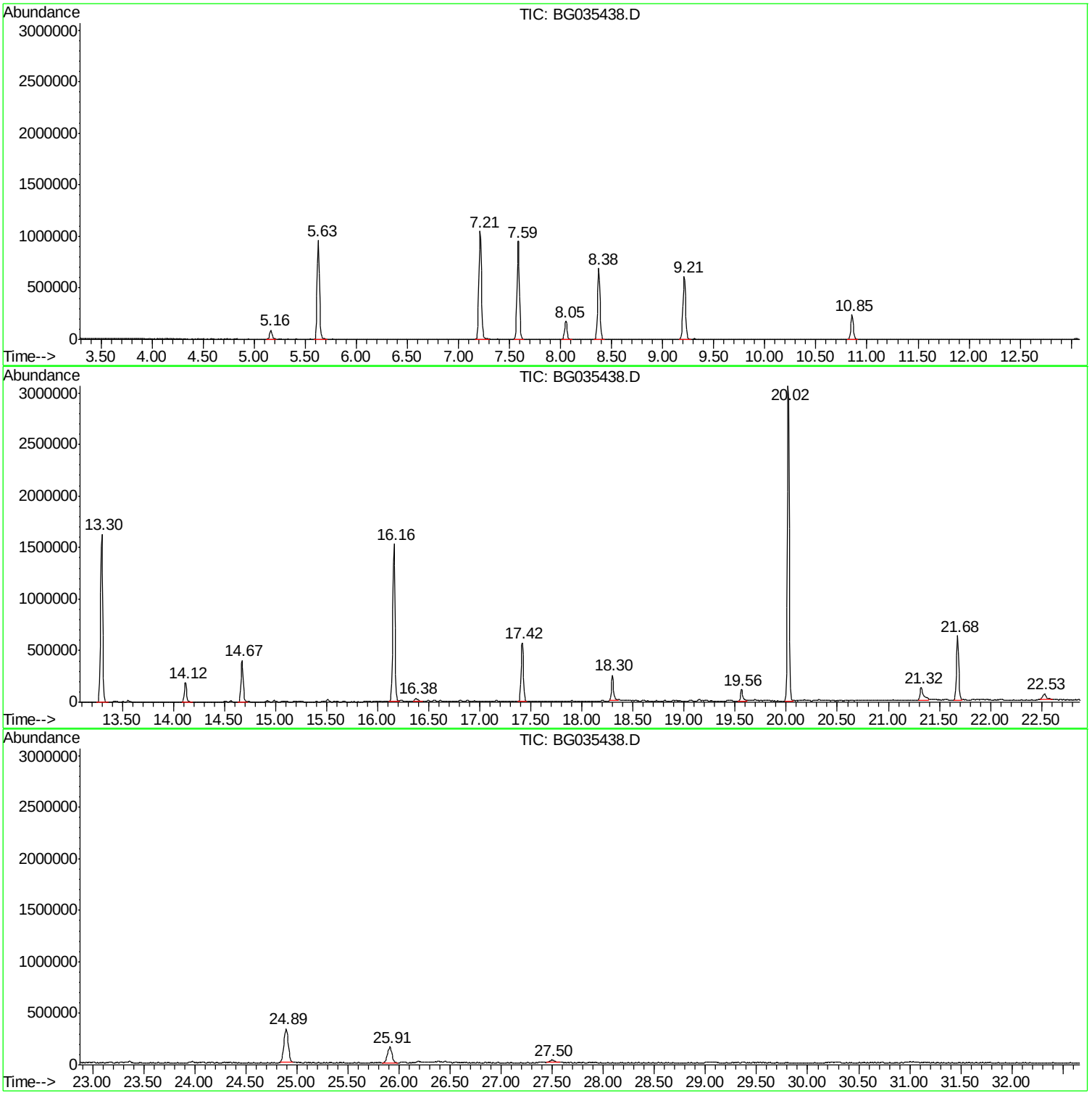
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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 G\DATA\BG062618\
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ClientSampleId : PE-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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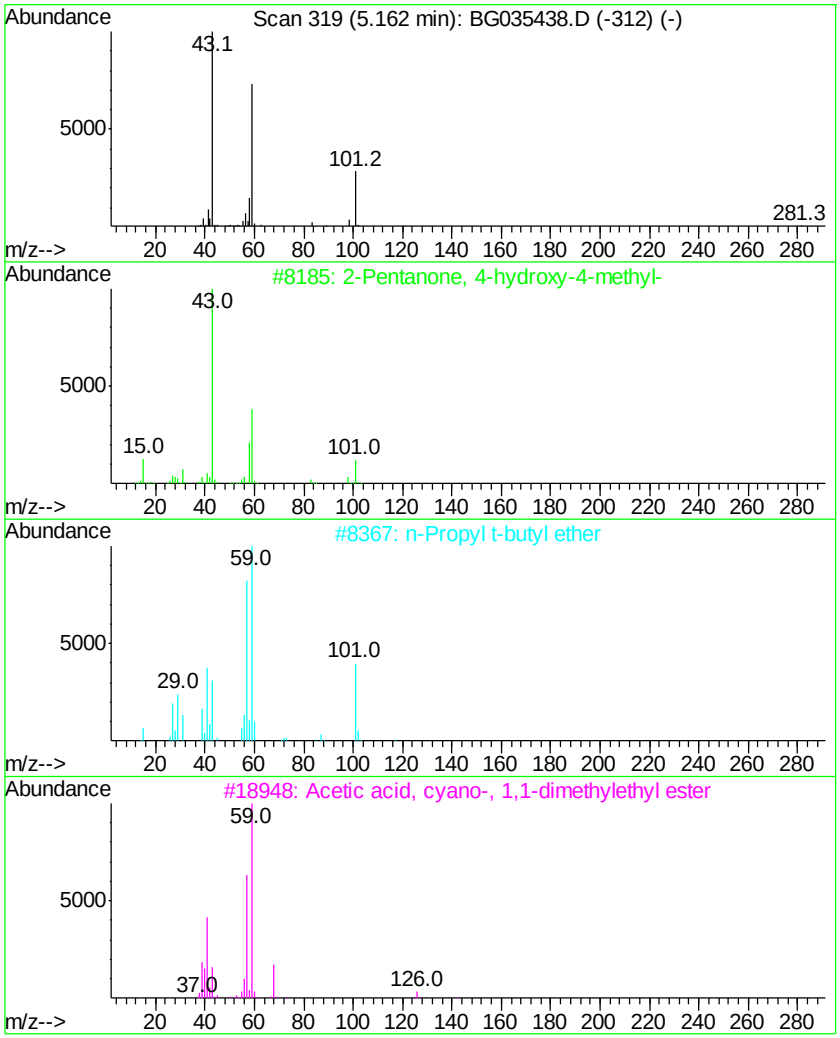
TIC Integration Parameters: LSCINT.P

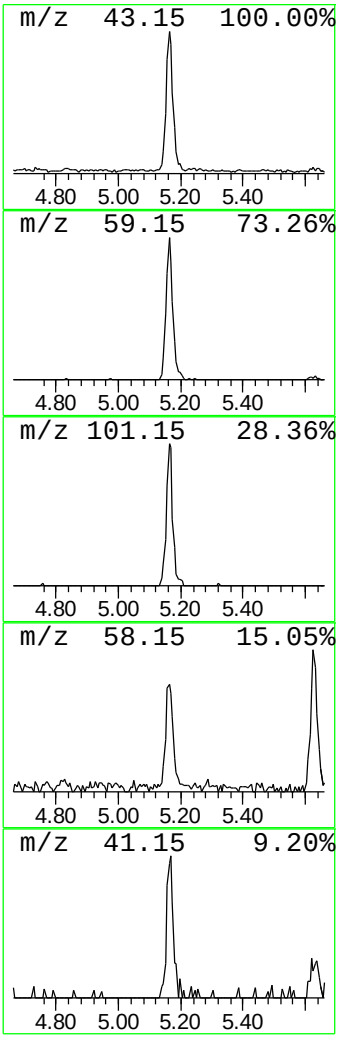
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	9.37 ng	141044	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	36
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
5	Propane, 2-methoxy-	74	C4H10O	000598-53-8	9





Library Search Compound Report

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Data File : BG035438.D
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Operator : JU/SJ
Sample : J3687-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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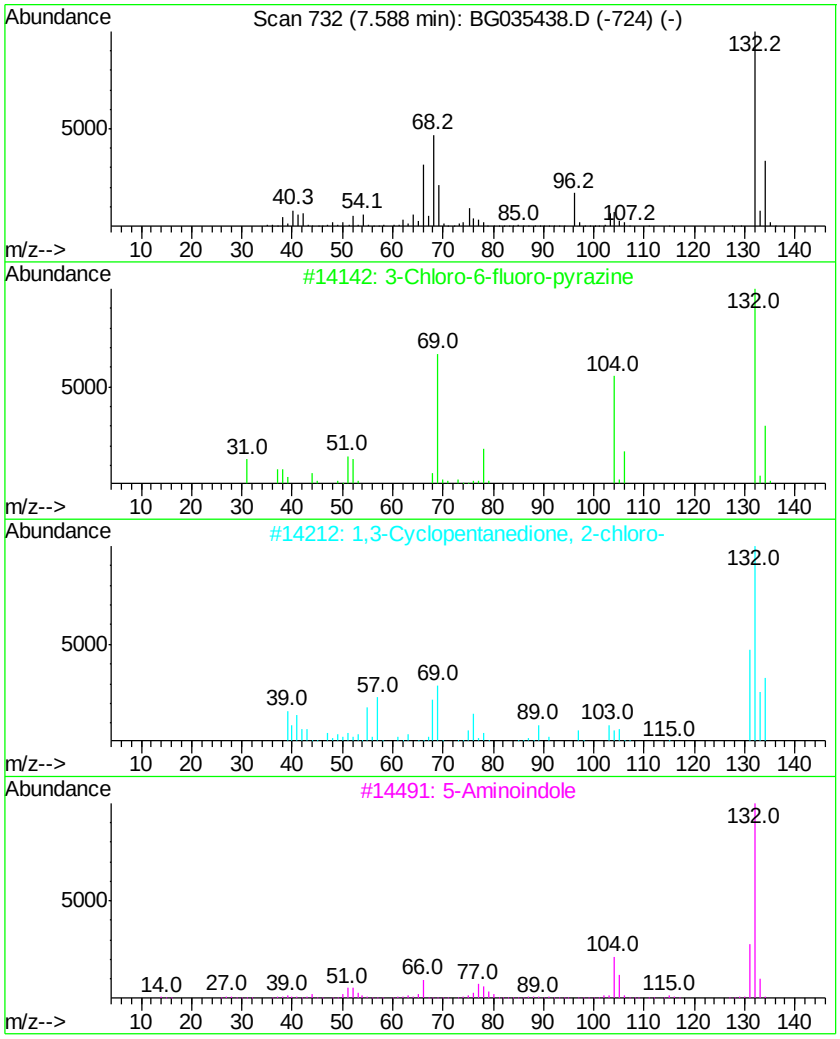
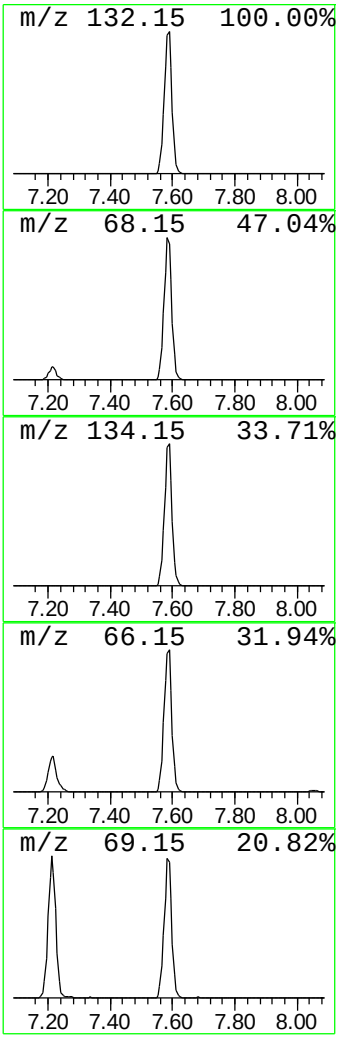
****

Peak Number 2 unknown7.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	111.59 ng	1680260	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062618\
Data File : BG035438.D
Acq On : 27 Jun 2018 9:49
Operator : JU/SJ
Sample : J3687-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

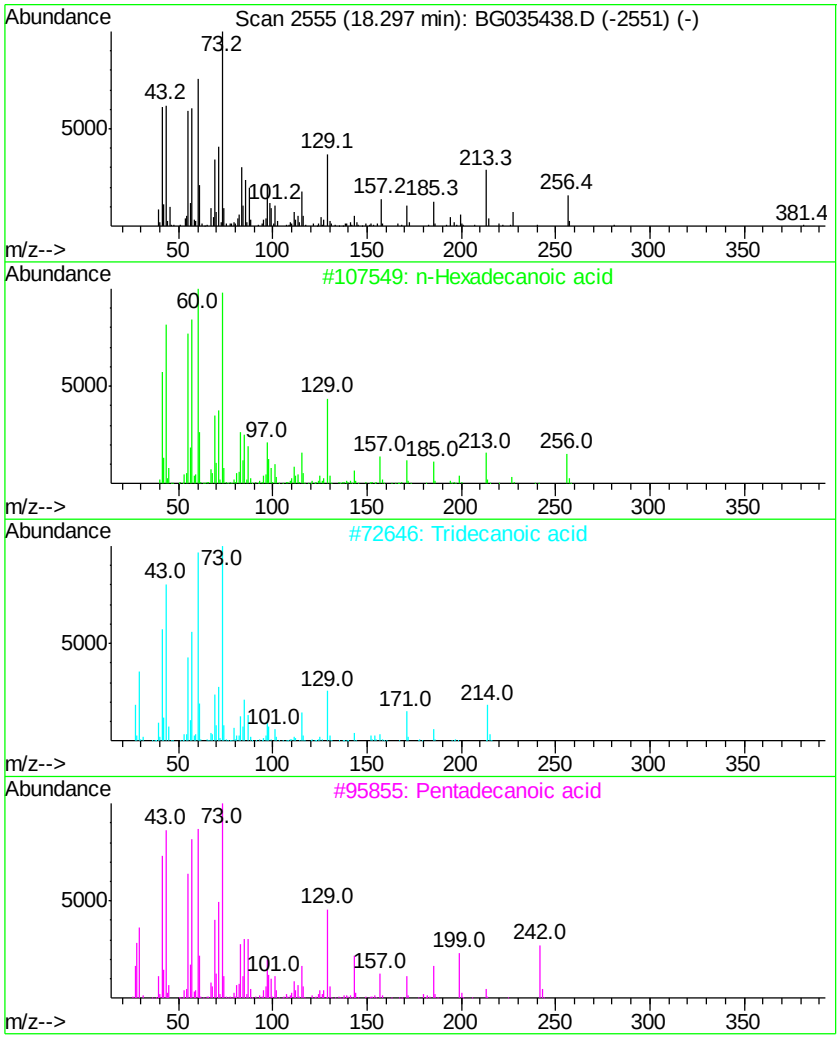
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

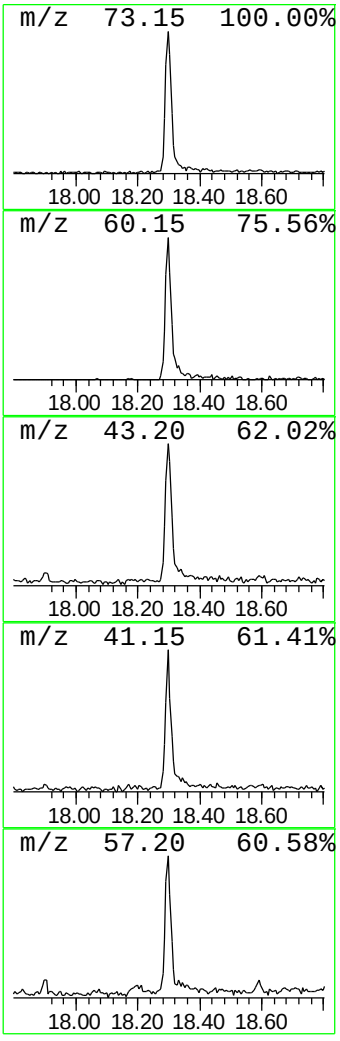
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	7.80 ng	345533	Phenanthrene-d10	17.42

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	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Octadecanoic acid	284	C18H36O2	000057-11-4	68
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





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Data File : BG035438.D
Acq On : 27 Jun 2018 9:49
Operator : JU/SJ
Sample : J3687-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

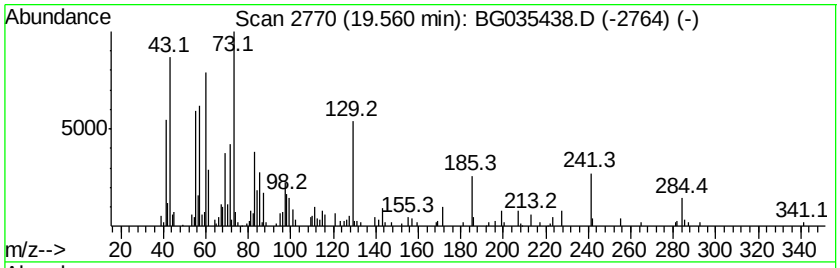
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

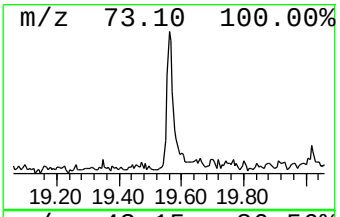
****

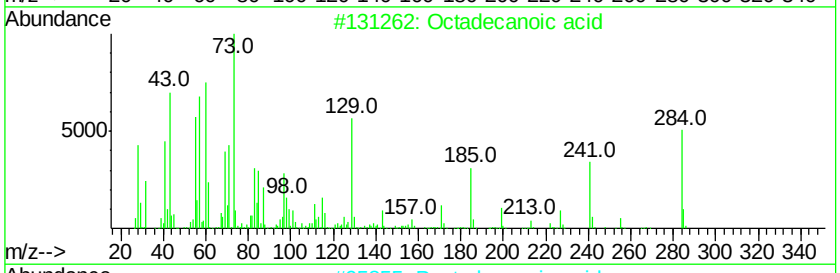
Peak Number 5 Octadecanoic acid Concentration Rank 7

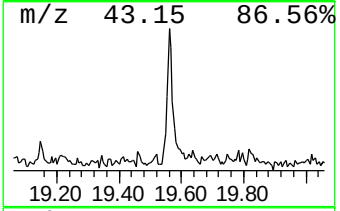
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.56	3.32 ng	172176	Chrysene-d12	21.68

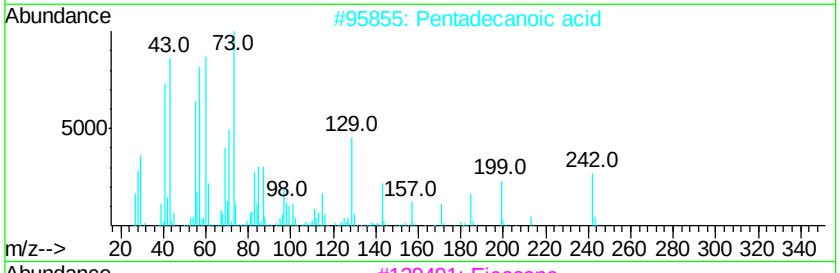
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
3	Eicosane	282	C20H42	000112-95-8	53
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
5	Undecanoic acid	186	C11H22O2	000112-37-8	30

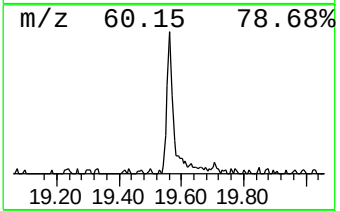


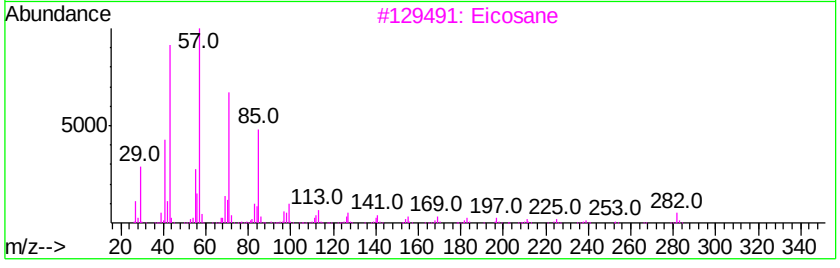


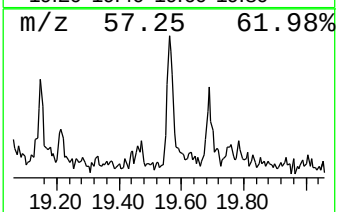


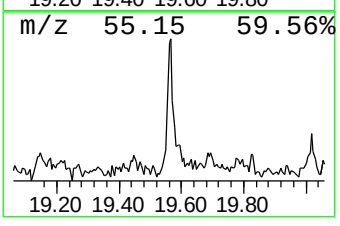












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ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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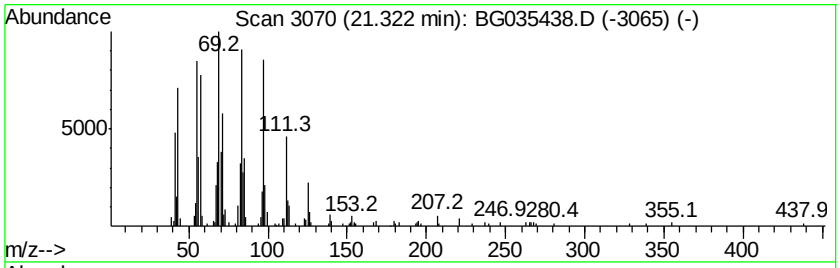
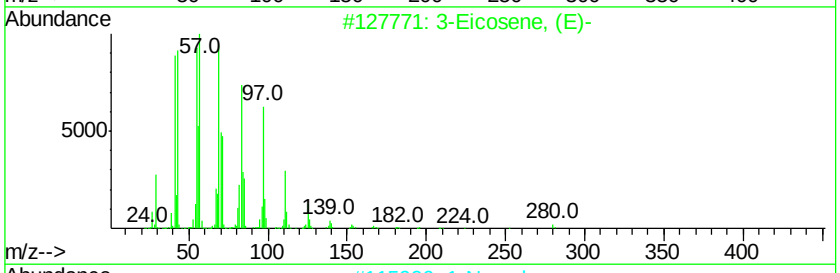
****

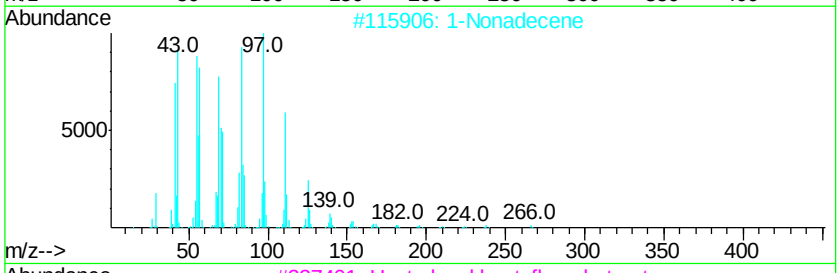
Peak Number 6 3-Eicosene, (E)- Concentration Rank 6

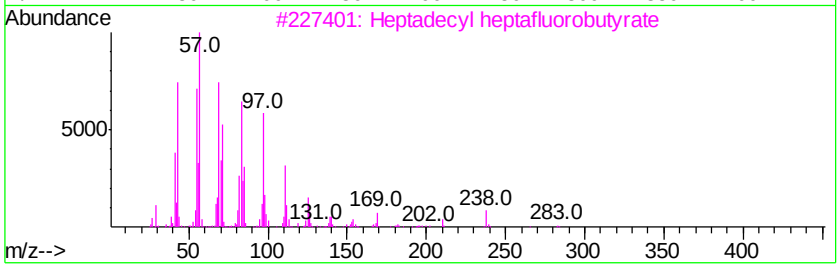
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.32	5.47 ng	283767	Chrysene-d12	21.68

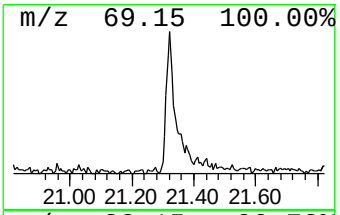
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	95
2	1-Nonadecene	266	C19H38	018435-45-5	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91

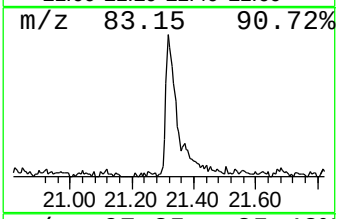


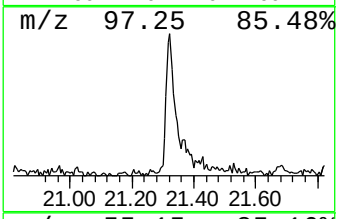


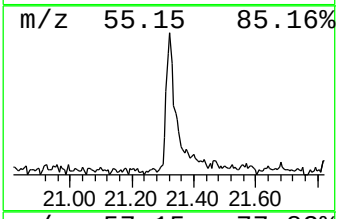


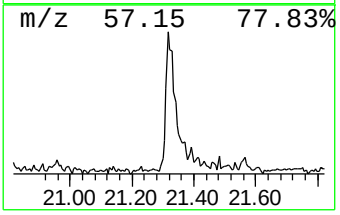












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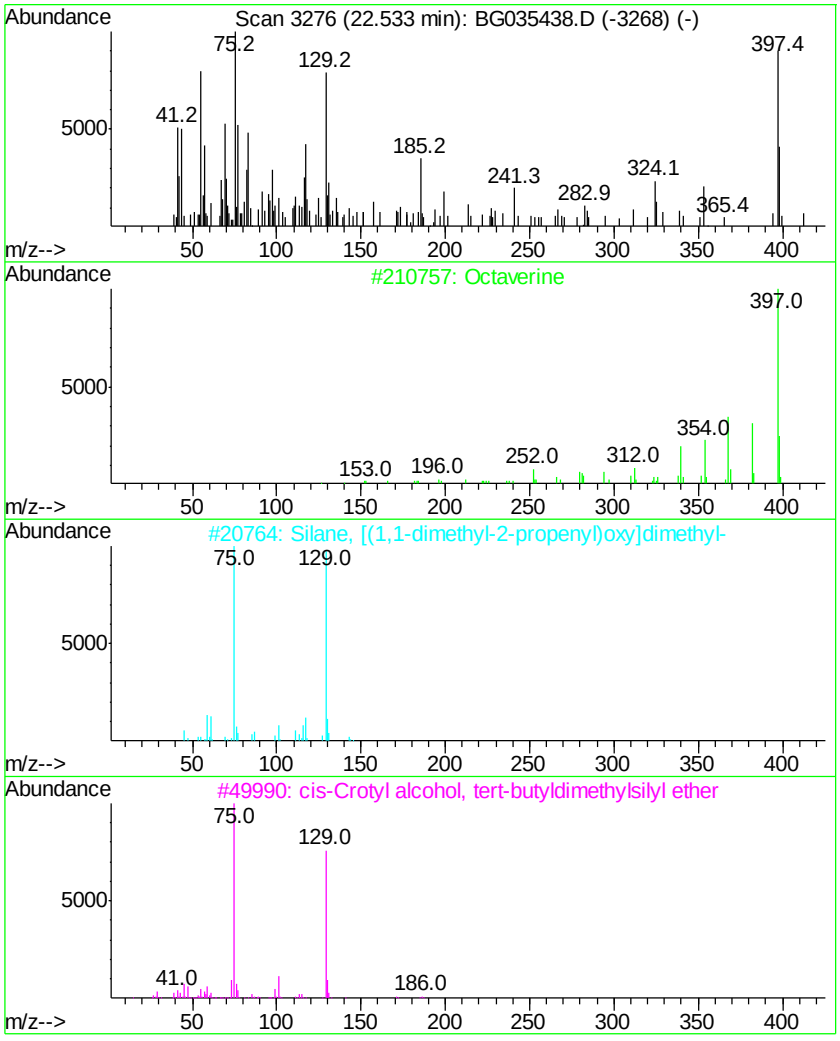
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

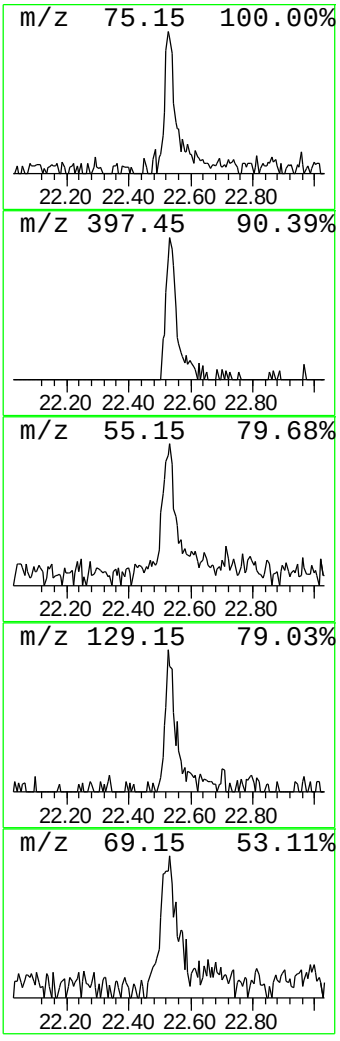
****

Peak Number 7 unknown22.53 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.53	2.77 ng	143573	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octaverine	397	C23H27NO5	000549-68-8	38
2	Silane, [(1,1-dimethyl-2-propenyl...	144	C7H16OSi	023483-22-9	38
3	cis-Crotyl alcohol, tert-butyldi...	186	C10H22OSi	1000333-02-2	35
4	2-Isopropyl(dimethyl)silyloxypro...	160	C8H20OSi	1000278-74-1	22
5	6b-Acetyl-4a,6a-dimethyl-3,4,4a,...	397	C26H39NO2	1000275-03-5	14





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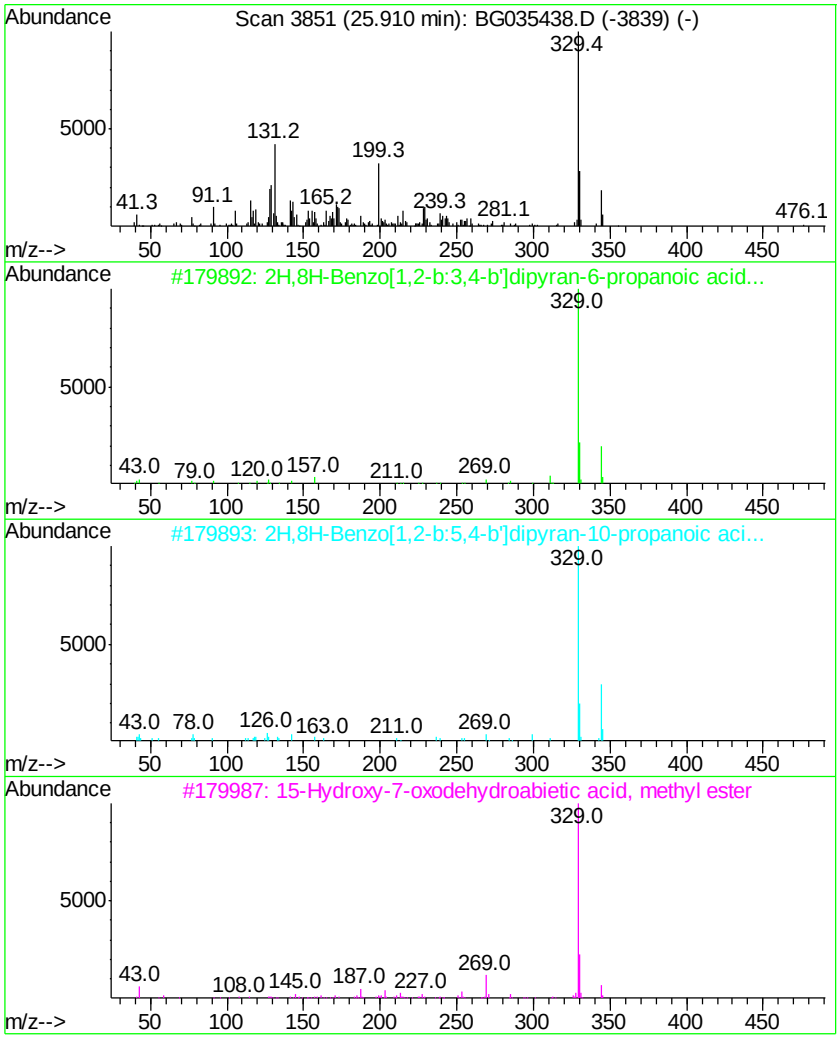
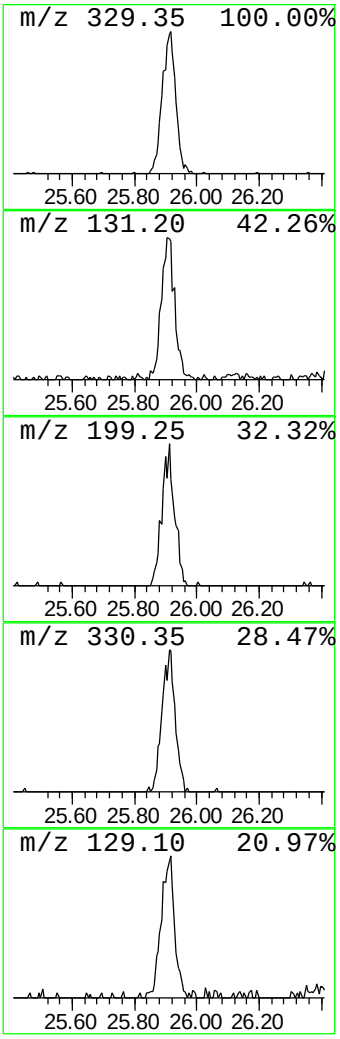
****

Peak Number 8 2H,8H-Benzo[1,2-b:3,4-b']di... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.91	10.23 ng	484329	Perylene-d12	24.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	344	C20H24O5	026535-36-4	50
2	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	344	C20H24O5	026535-35-3	38
3	15-Hydroxy-7-oxodehydroabietic a...	344	C21H28O4	060188-95-6	32
4	Silylamine, 1,1,1-trimethyl-N-[4...	329	C18H27NOSi2	031396-30-2	30
5	1-Hydroxy-4-(p-toluidino)anthraq...	329	C21H15NO3	000081-48-1	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG062618\
Data File : BG035438.D
Acq On : 27 Jun 2018 9:49
Operator : JU/SJ
Sample : J3687-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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...	5.16	9.4	ng	141044	1	8.05	301154	20.0
unknown7.59	7.59	111.6	ng	1680260	1	8.05	301154	20.0
n-Hexadecanoic acid	18.30	7.8	ng	345533	4	17.42	885559	20.0
Octadecanoic acid	19.56	3.3	ng	172176	5	21.68	1037080	20.0
3-Eicosene, (E)-	21.32	5.5	ng	283767	5	21.68	1037080	20.0
unknown22.53	22.53	2.8	ng	143573	5	21.68	1037080	20.0
2H,8H-Benzo[1,2-b...	25.91	10.2	ng	484329	6	24.89	946997	20.0