LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG092518\
Data File : BG036954.D
Acq On : 25 Sep 2018 18:19
Operator : JU/SJ
Sample : J5055-12
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-C

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-BG092018.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	5.150	311	317	324	rBV	36051	59206	2.32%	0.349%
2	5.614	390	396	411	rBV	728115	1295804	50.80%	7.632%
3	7.206	659	667	682	rBV	713359	1459379	57.22%	8.595%
4	7.576	721	730	746	rBV	695044	1354121	53.09%	7.975%
5	8.040	803	809	818	rBV2	145388	279396	10.95%	1.646%
6	8.363	855	864	880	rBV	551467	1029941	40.38%	6.066%
7	9.204	998	1007	1023	rBV	443474	902227	35.37%	5.314%
8	10.843	1279	1286	1296	rBV	191060	388025	15.21%	2.285%
9	13.293	1695	1703	1716	rBV	1140679	1918338	75.21%	11.298%
10	14.116	1833	1843	1854	rBV	325662	529060	20.74%	3.116%
11	14.492	1904	1907	1914	rVB3	19601	33735	1.32%	0.199%
12	14.668	1925	1937	1947	rBV2	335093	615357	24.13%	3.624%
13	15.379	2054	2058	2065	rBV7	14991	33926	1.33%	0.200%
14	15.455	2066	2071	2077	rBV5	43283	75304	2.95%	0.444%
15	16.154	2184	2190	2201	rBV	1000881	1664559	65.26%	9.803%
16	17.412	2399	2404	2412	rBV2	403707	662554	25.98%	3.902%
17	18.293	2551	2554	2561	rBV6	62817	121930	4.78%	0.718%
18	20.020	2842	2848	2857	rBV	1891995	2550555	100.00%	15.022%
19	21.319	3065	3069	3074	rBV3	37887	63573	2.49%	0.374%
20	21.677	3124	3130	3143	rVB2	470828	834985	32.74%	4.918%
21	23.158	3378	3382	3388	rVB3	26716	51154	2.01%	0.301%
22	23.346	3408	3414	3422	rVB	72917	139126	5.45%	0.819%
23	23.957	3513	3518	3525	rVB3	28782	59400	2.33%	0.350%
24	24.885	3666	3676	3688	rVB	281862	857667	33.63%	5.051%

Sum of corrected areas: 16979322

LSC Report - Integrated Chromatogram

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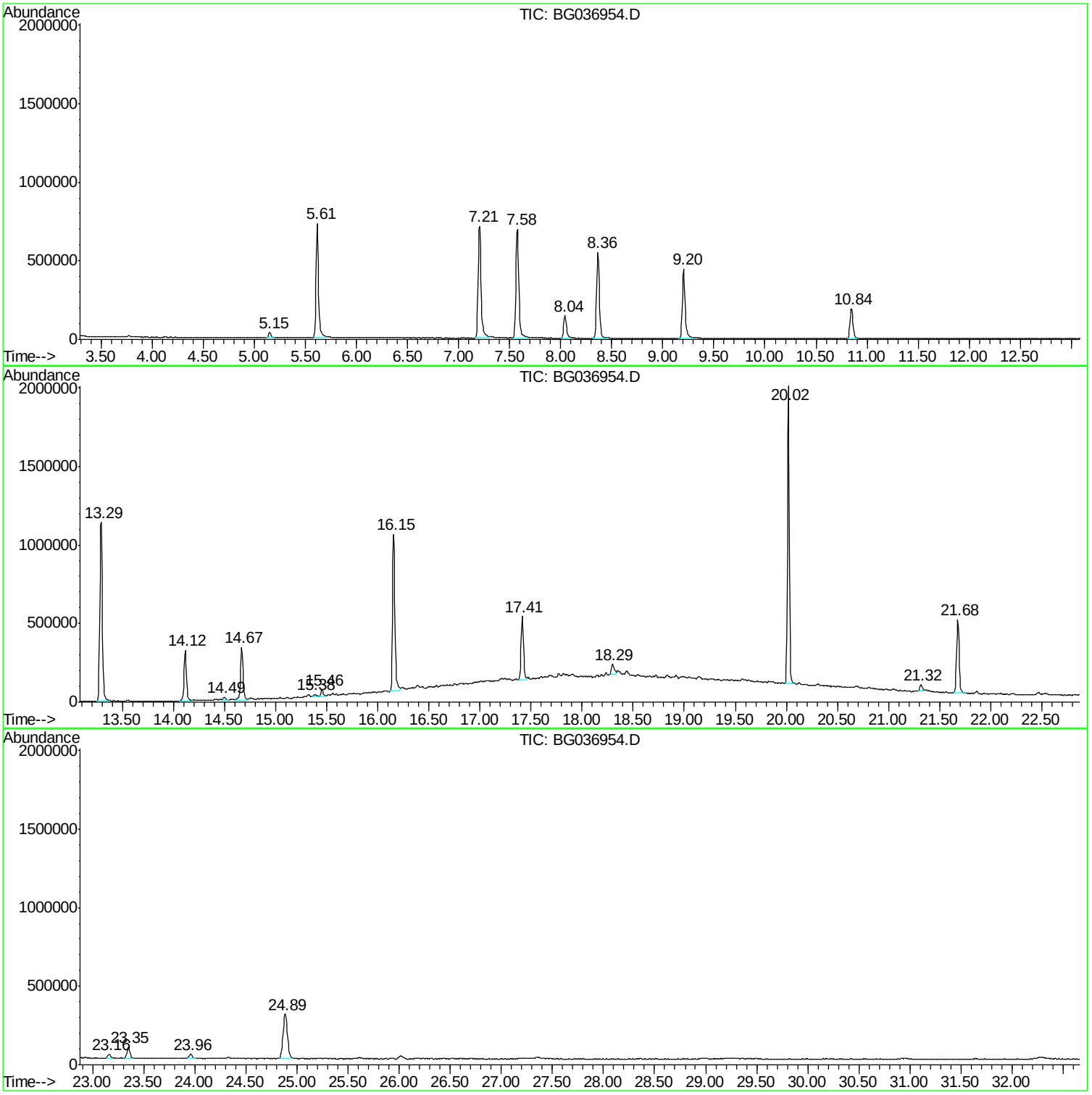
Instrument : BNA_G
ClientSampleId : TP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.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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Instrument : BNA_G
ClientSampleId : TP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.M
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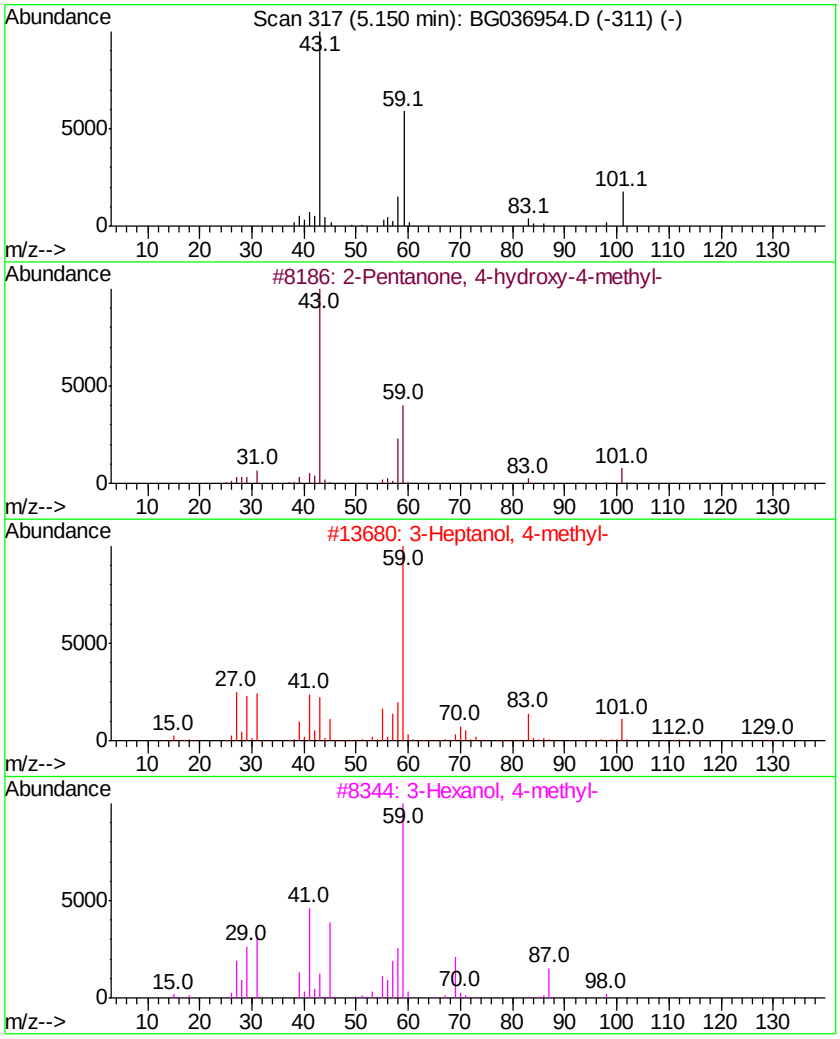
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

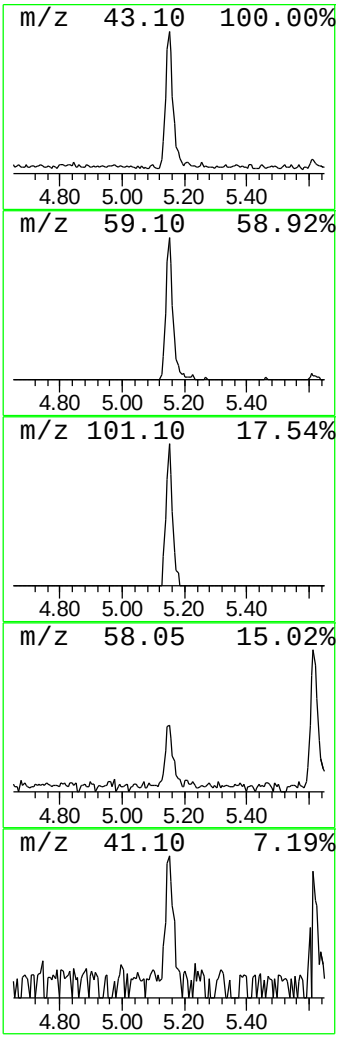
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	4.24 ng	59206	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	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	28
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5	3-Heptanol	116	C7H16O	000589-82-2	25





Library Search Compound Report

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ClientSampleId : TP-C

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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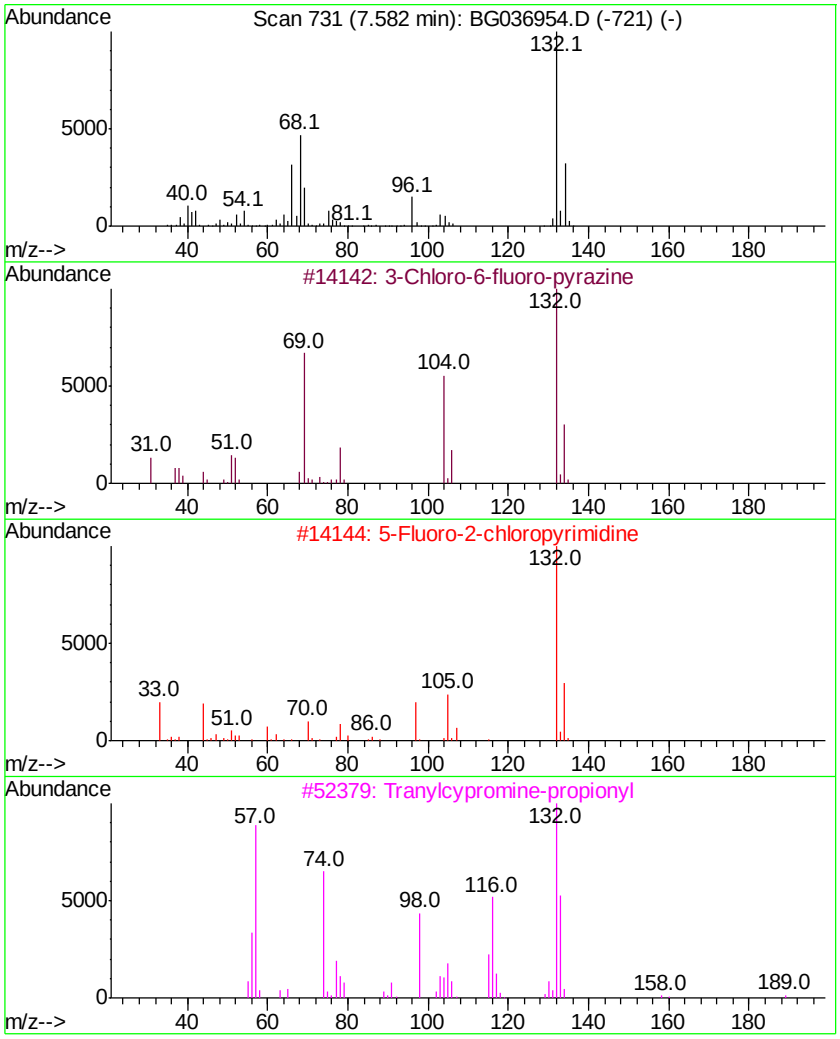
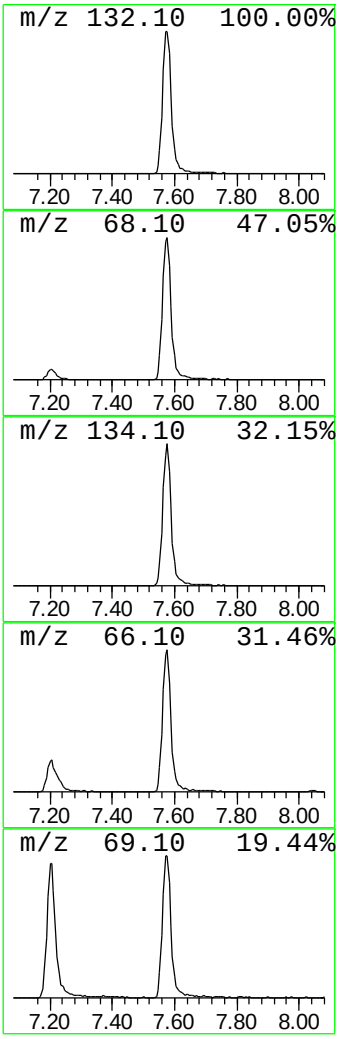
Peak Number 2 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	96.93 ng	1354120	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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5	N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10





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Instrument : BNA_G
ClientSampleId : TP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.M
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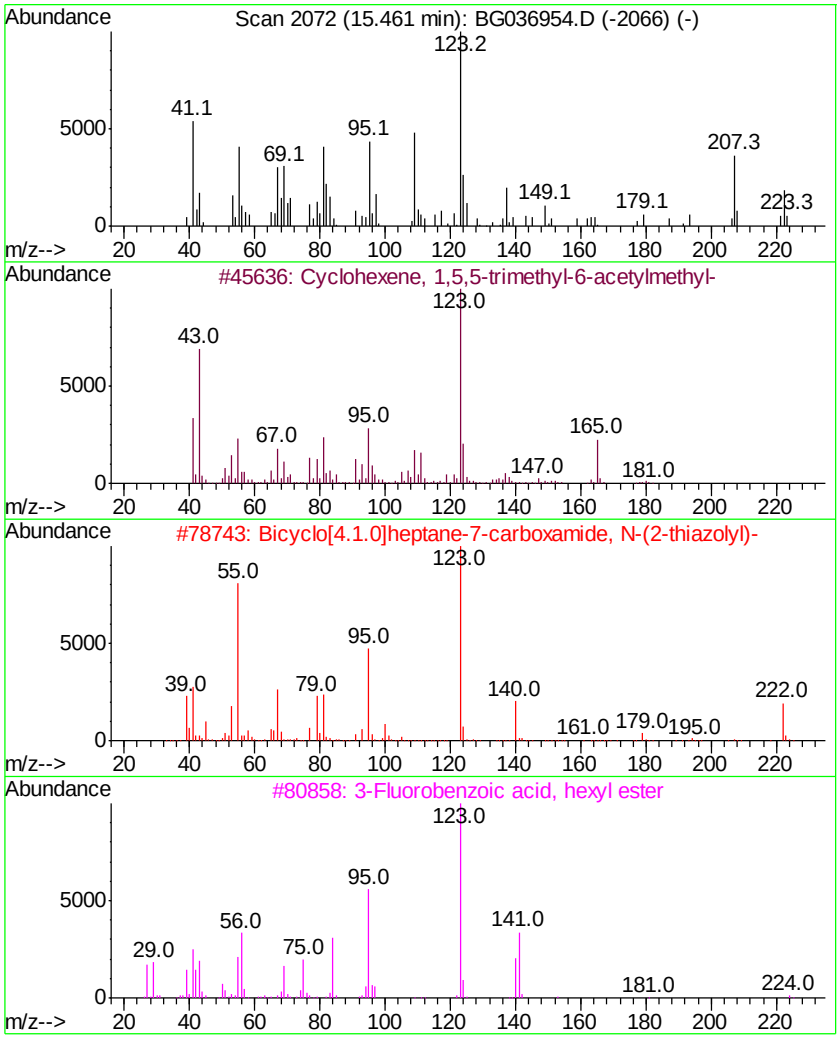
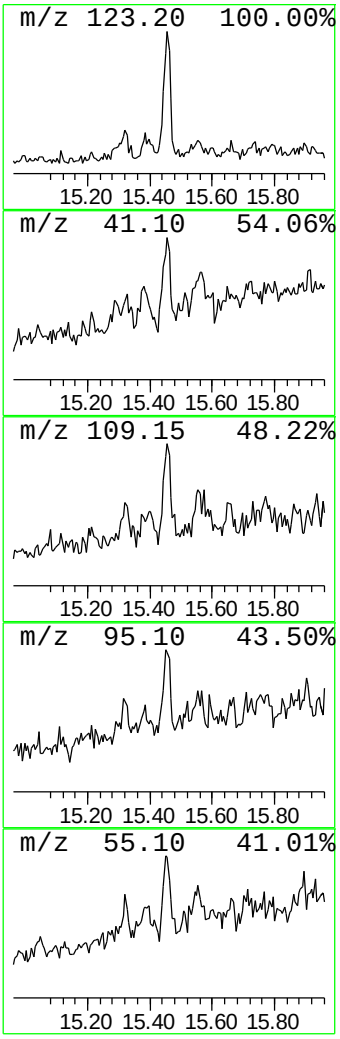
Peak Number 4 unknown15.46 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.46	2.45 ng	75304	Acenaphthene-d10	14.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 1,5,5-trimethyl-6-a...	180	C12H20O	211563-96-1	47
2	Bicyclo[4.1.0]heptane-7-carboxam...	222	C11H14N2OS	329912-72-3	38
3	3-Fluorobenzoic acid, hexyl ester	224	C13H17FO2	1000279-00-8	38
4	2-Fluorobenzoic acid, 3-tetradec...	336	C21H33FO2	1000280-61-3	38
5	4-Fluorobenzoic acid, 3-pentadec...	350	C22H35FO2	1000280-68-4	38





Library Search Compound Report

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ClientSampleId : TP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.M
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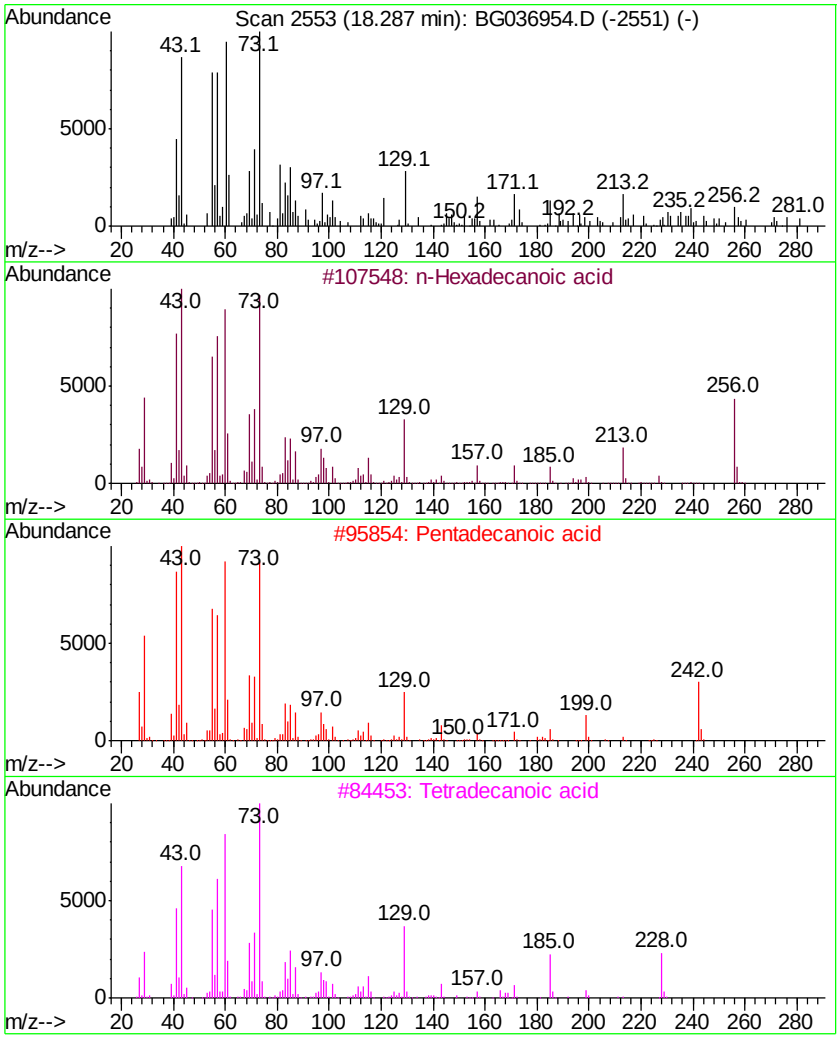
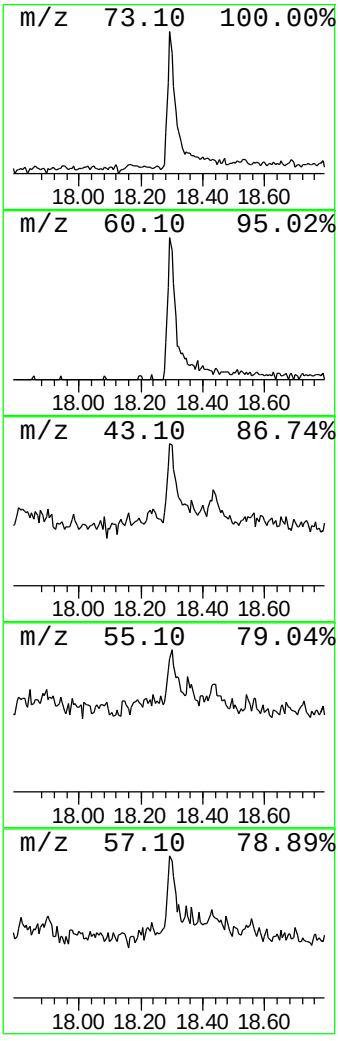
Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.29	3.68 ng	121930	Phenanthrene-d10	17.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	12-Bromododecanoic acid	278	C12H23BrO2	073367-80-3	47





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ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-C

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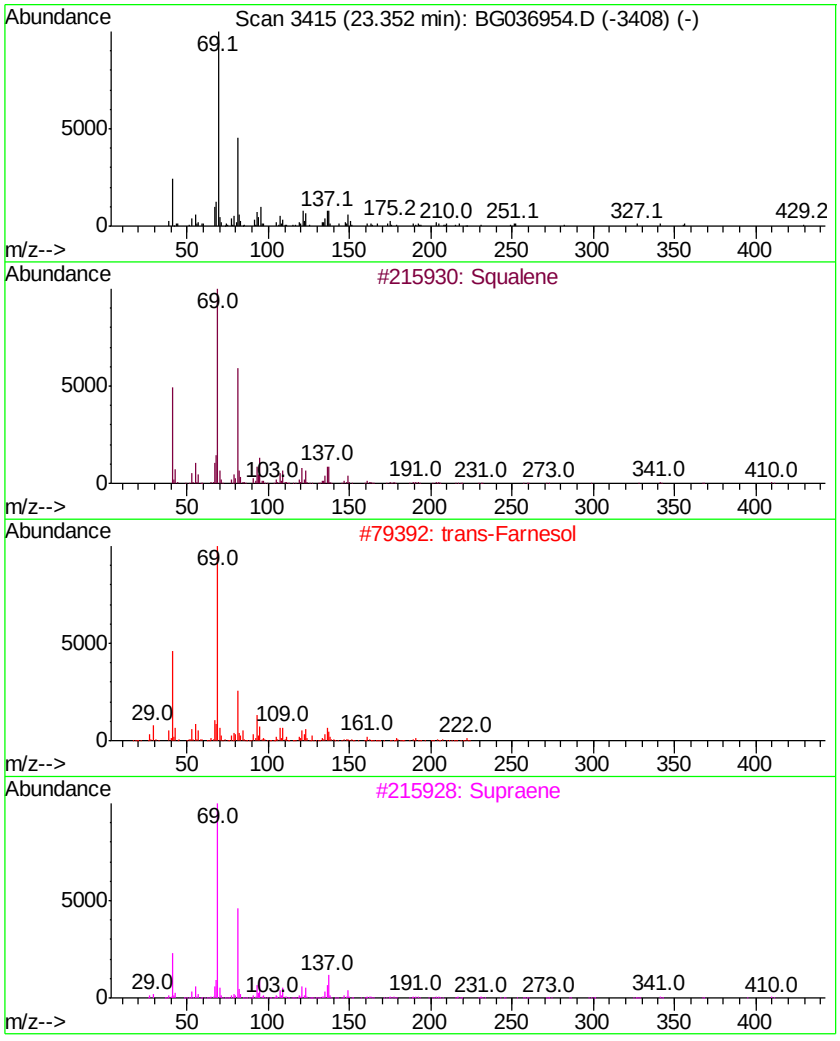
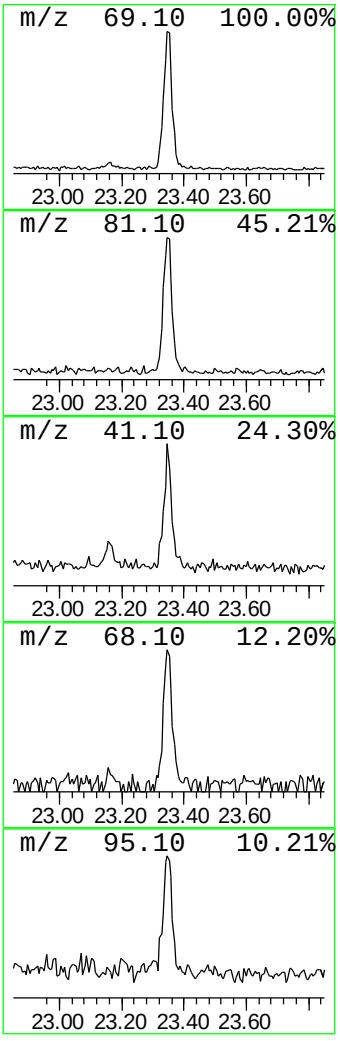
****

Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.35	3.24 ng	139126	Perylene-d12	24.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	87
2	trans-Farnesol	222	C15H26O	000106-28-5	72
3	Supraene	410	C30H50	007683-64-9	72
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.15	4.2	ng	59206	1	8.05	279396	20.0
unknown7.58	7.58	96.9	ng	1354120	1	8.05	279396	20.0
unknown15.46	15.46	2.5	ng	75304	3	14.67	615357	20.0
n-Hexadecanoic acid	18.29	3.7	ng	121930	4	17.41	662554	20.0
Squalene	23.35	3.2	ng	139126	6	24.88	857667	20.0