LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG012117\
Data File : BG025582.D
Acq On : 21 Jan 2017 20:46
Operator : UM/SJ
Sample : I1271-03
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SS-02

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_G\METHODS\8270-BG122116.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	5.235	402	408	417	rBV	683963	1125116	14.78%	2.817%
2	5.717	484	490	502	rBV	1533449	2629760	34.55%	6.583%
3	7.339	759	766	785	rBV	1607337	3107848	40.83%	7.780%
4	7.709	822	829	839	rBV	1611028	2880235	37.84%	7.210%
5	8.179	902	909	922	rVB	335449	613063	8.05%	1.535%
6	8.502	957	964	973	rBV	1234433	2175632	28.58%	5.446%
7	9.366	1102	1111	1123	rBV	1002608	1960159	25.75%	4.907%
8	11.005	1382	1390	1400	rBV	443438	852082	11.20%	2.133%
9	13.426	1795	1802	1811	rBV	2693747	4361325	57.30%	10.918%
10	14.248	1937	1942	1949	rVB	184848	303777	3.99%	0.760%
11	14.806	2031	2037	2044	rVB	763080	1238374	16.27%	3.100%
12	15.993	2233	2239	2244	rVB4	65602	119731	1.57%	0.300%
13	16.299	2284	2291	2305	rBV	2831121	4452874	58.50%	11.147%
14	16.475	2313	2321	2325	rBV3	110234	247607	3.25%	0.620%
15	17.245	2449	2452	2456	rVB2	70155	85731	1.13%	0.215%
16	17.298	2456	2461	2466	rBV4	52108	84587	1.11%	0.212%
17	17.556	2499	2505	2513	rBV	1038459	1645449	21.62%	4.119%
18	18.396	2644	2648	2659	rBV3	158034	270960	3.56%	0.678%
19	20.135	2938	2944	2950	rBV	5469001	7611262	100.00%	19.054%
20	21.410	3157	3161	3162	rBV3	103619	114964	1.51%	0.288%
21	21.845	3228	3235	3244	rVB	1187156	2055964	27.01%	5.147%
22	25.229	3802	3811	3825	rVB2	672496	2009241	26.40%	5.030%

Sum of corrected areas: 39945741

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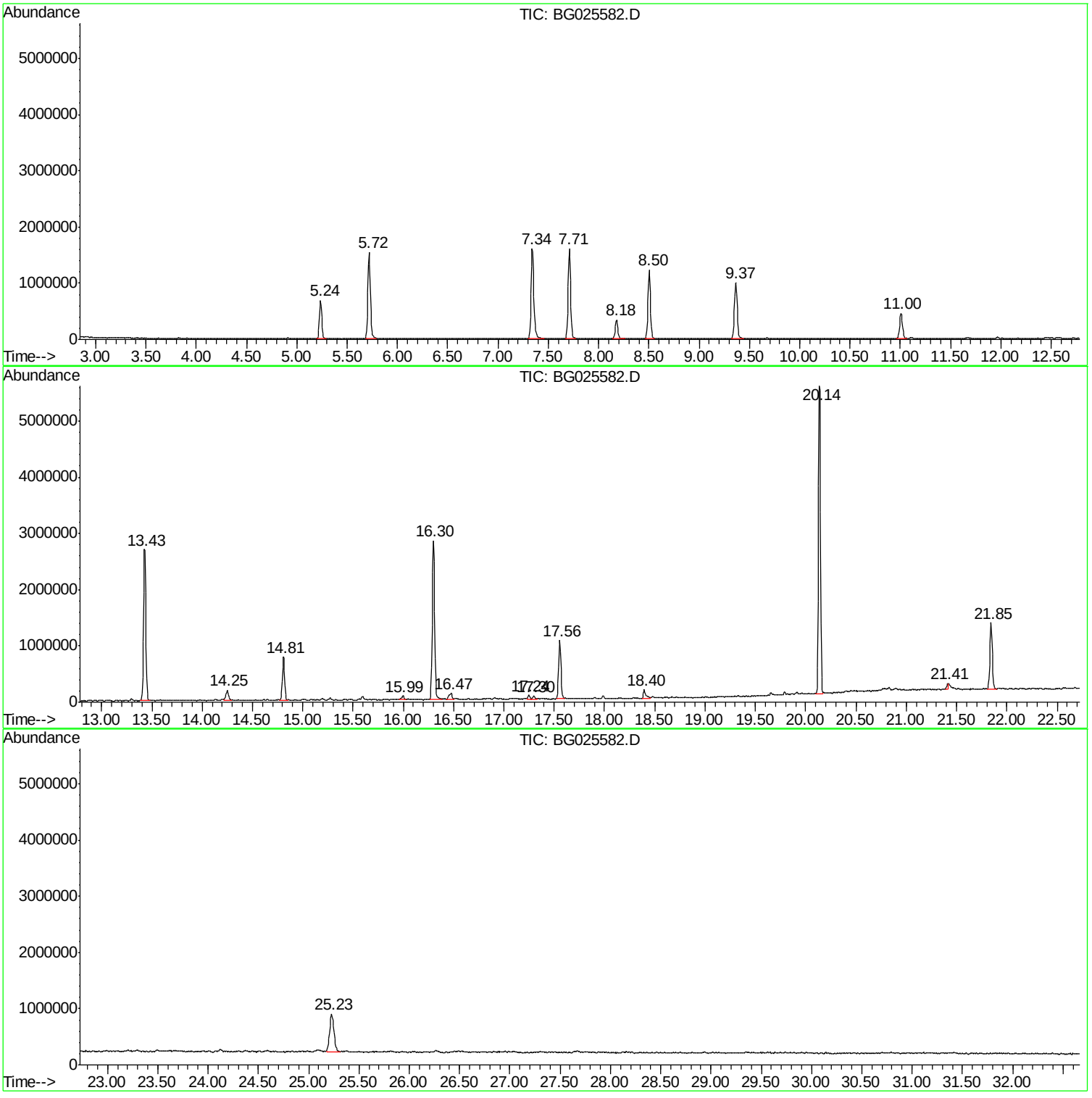
ClientSampleId : SS-02

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.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 : BG025582.D
Acq On : 21 Jan 2017 20:46
Operator : UM/SJ
Sample : I1271-03
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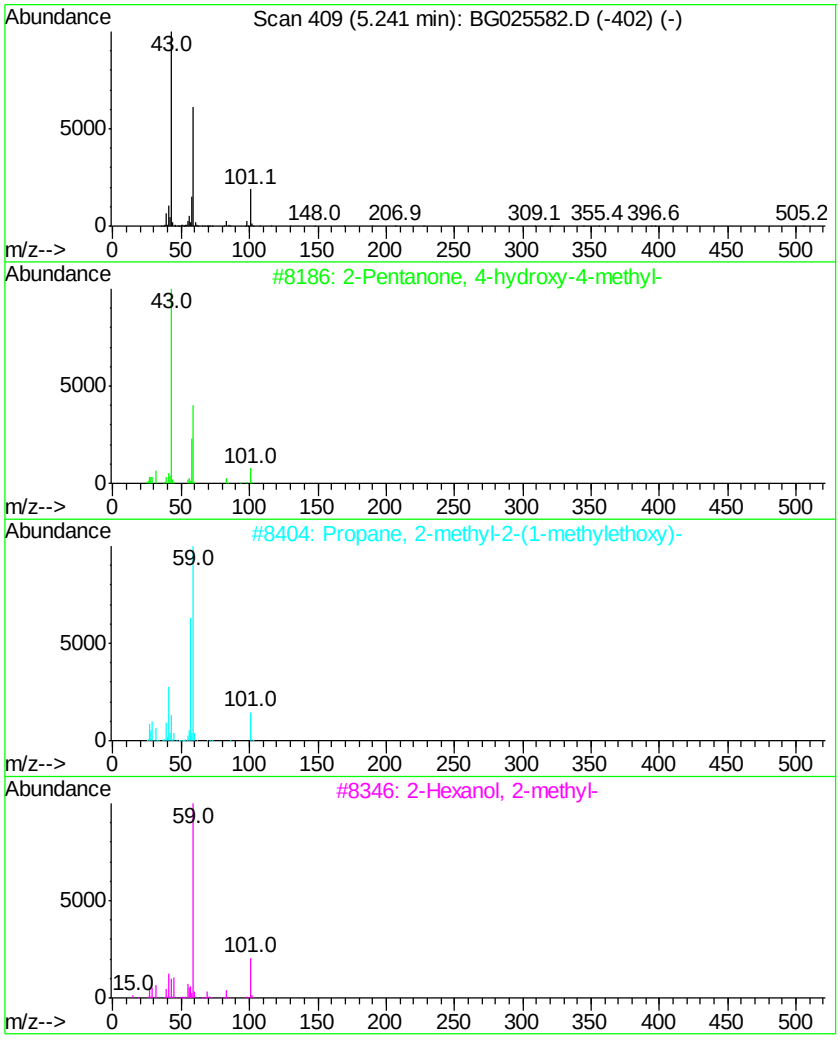
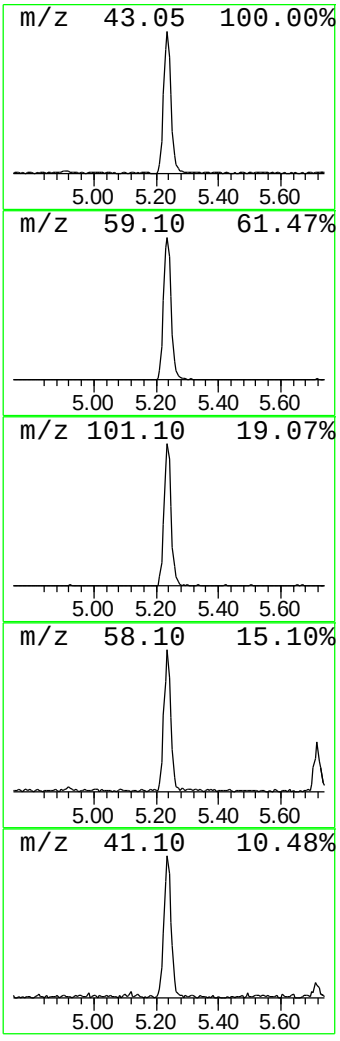
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	36.70 ng	1125120	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Library Search Compound Report

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ClientSampleId : SS-02

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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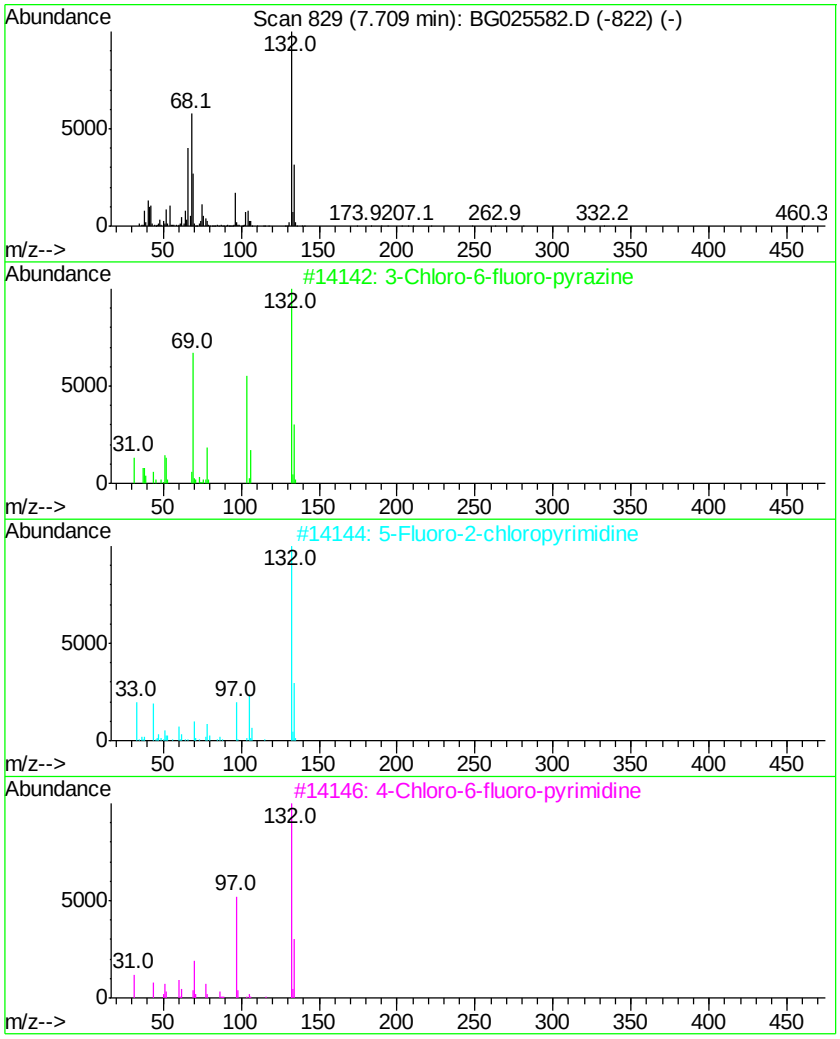
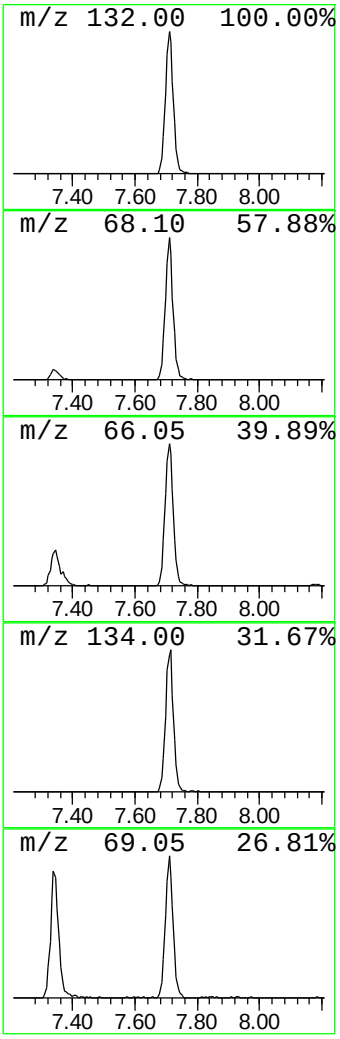
Peak Number 2 unknown7.71 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.71	93.96 ng	2880240	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10





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Data File : BG025582.D
Acq On : 21 Jan 2017 20:46
Operator : UM/SJ
Sample : I1271-03
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SS-02

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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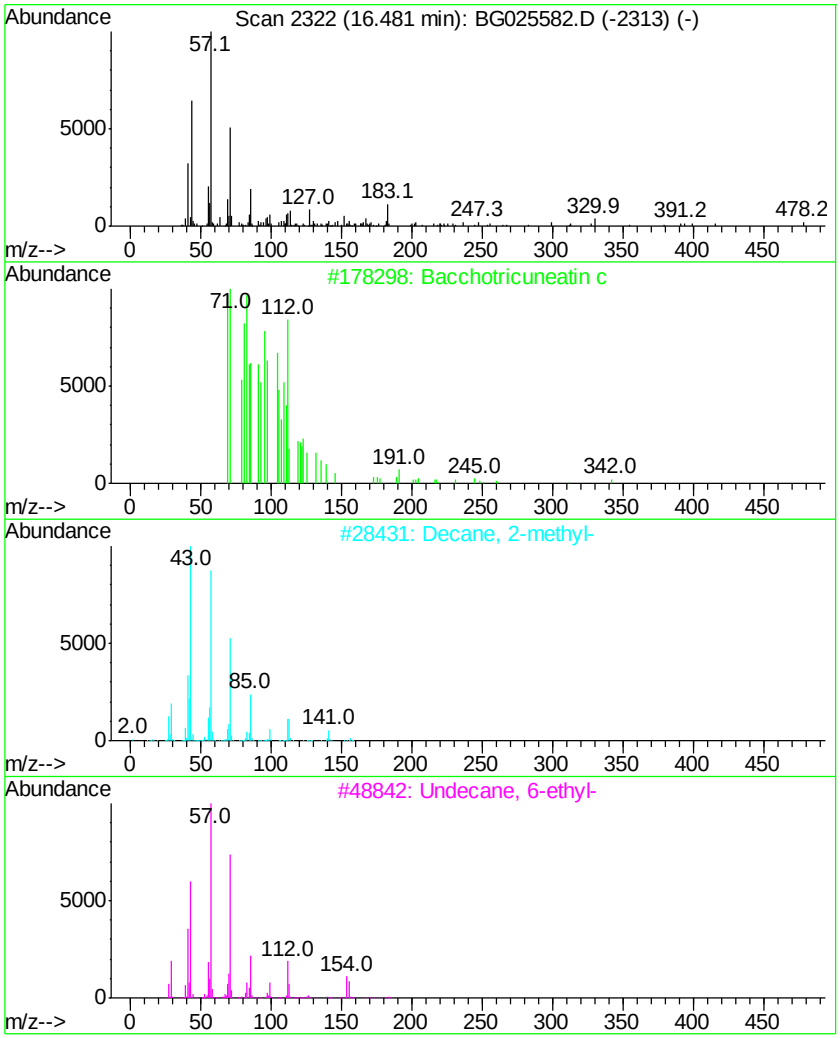
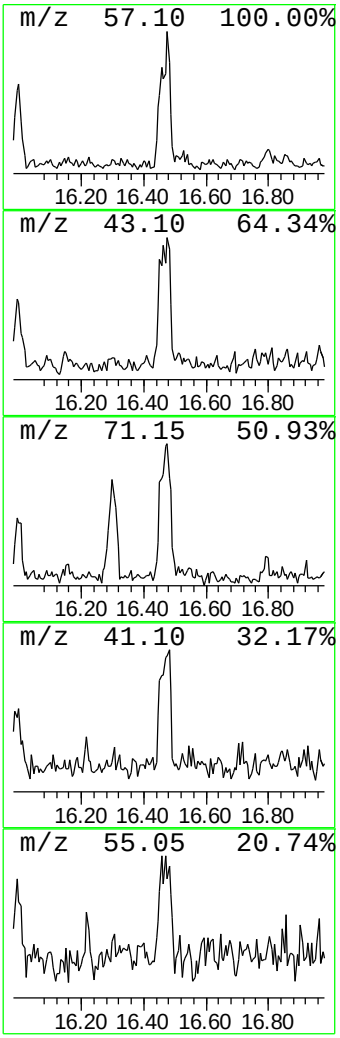
Peak Number 4 Bacchotricuneatin c Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.48	3.01 ng	247607	Phenanthrene-d10	17.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bacchotricuneatin c	342	C20H22O5	066563-30-2	95
2	Decane, 2-methyl-	156	C11H24	006975-98-0	83
3	Undecane, 6-ethyl-	184	C13H28	017312-60-6	83
4	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	80
5	Hexadecane, 7-methyl-	240	C17H36	026730-20-1	72





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ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SS-02

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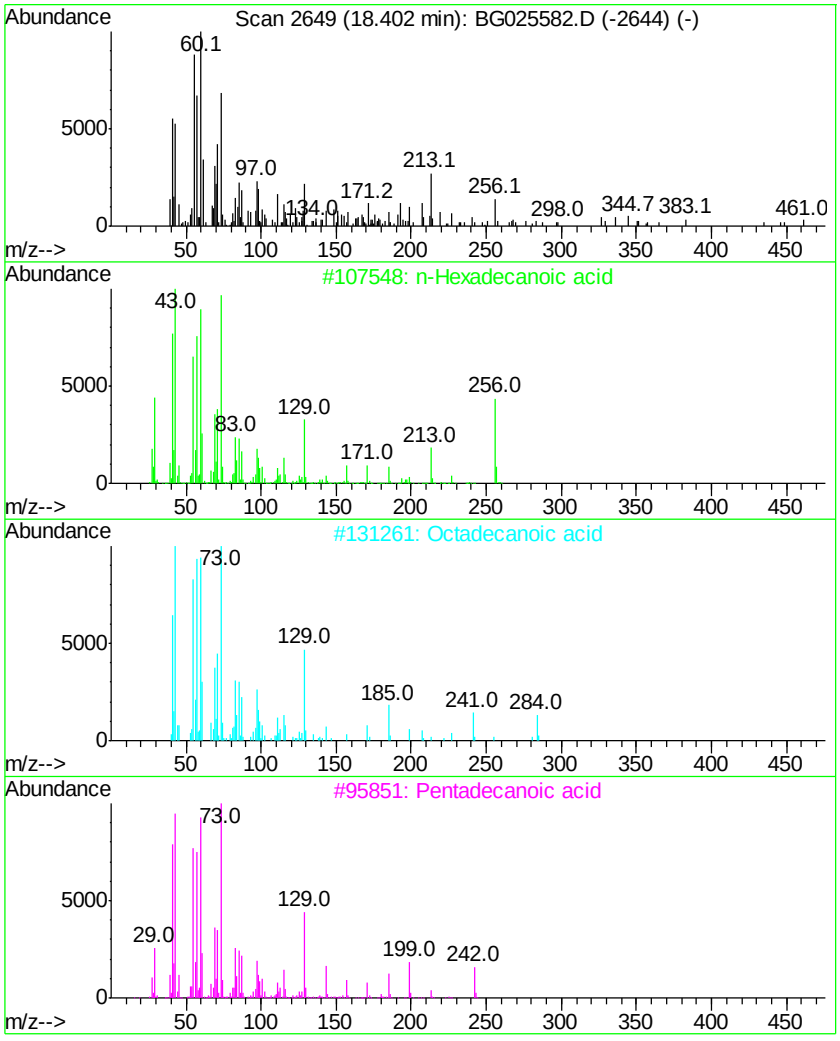
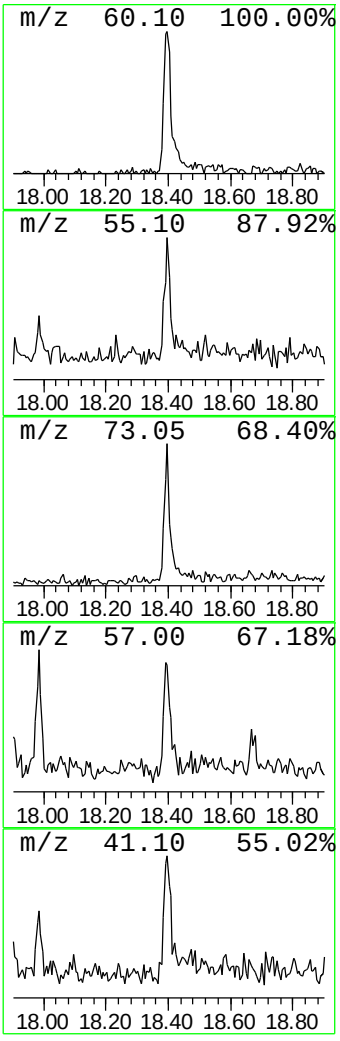
Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.40	3.29 ng	270960	Phenanthrene-d10	17.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
2	Octadecanoic acid	284	C18H36O2	000057-11-4	64
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG012117\
Data File : BG025582.D
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Operator : UM/SJ
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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...	5.24	36.7	ng	1125120	1	8.17	613063	20.0
unknown7.71	7.71	94.0	ng	2880240	1	8.17	613063	20.0
Bacchotricuneatin c	16.48	3.0	ng	247607	4	17.56	1645450	20.0
n-Hexadecanoic acid	18.40	3.3	ng	270960	4	17.56	1645450	20.0