LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG101717\
Data File : BG029307.D
Acq On : 17 Oct 2017 18:53
Operator : SJ/JU
Sample : I5821-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : WPSB-6B-18-18.5-BGS

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-BG101617.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	5.242	327	332	345	rBV	155934	249672	6.77%	1.122%
2	5.718	406	413	428	rBV	894174	1463307	39.67%	6.578%
3	7.322	678	686	700	rBV	970225	1768823	47.95%	7.952%
4	7.698	742	750	765	rBV	928470	1618251	43.87%	7.275%
5	8.168	822	830	837	rBV	196130	329060	8.92%	1.479%
6	8.497	878	886	894	rVB	664372	1151447	31.21%	5.176%
7	9.331	1020	1028	1037	rBV	560554	1018417	27.61%	4.578%
8	10.988	1302	1310	1321	rVB	295529	529896	14.37%	2.382%
9	12.280	1523	1530	1539	rBV	85827	140448	3.81%	0.631%
10	13.414	1716	1723	1731	rBV	1707553	2595324	70.36%	11.667%
11	14.225	1855	1861	1869	rBV	238970	356086	9.65%	1.601%
12	14.789	1950	1957	1966	rVB2	496569	803649	21.79%	3.613%
13	16.129	2179	2185	2193	rBV	458168	661962	17.95%	2.976%
14	16.270	2202	2209	2220	rBV	1421470	2186796	59.28%	9.831%
15	17.521	2416	2422	2431	rVB2	656319	997939	27.05%	4.486%
16	18.391	2562	2570	2577	rBV	85630	121843	3.30%	0.548%
17	19.654	2780	2785	2791	rBV3	39777	59566	1.61%	0.268%
18	19.801	2806	2810	2815	rBV	53044	58062	1.57%	0.261%
19	20.112	2857	2863	2870	rBV	2844198	3688797	100.00%	16.583%
20	20.835	2982	2986	2992	rBV	37739	44150	1.20%	0.198%
21	21.417	3081	3085	3091	rBV3	58715	94921	2.57%	0.427%
22	21.793	3142	3149	3162	rVB2	684868	1170214	31.72%	5.261%
23	25.101	3701	3712	3727	rBV2	347190	1136305	30.80%	5.108%

Sum of corrected areas: 22244935

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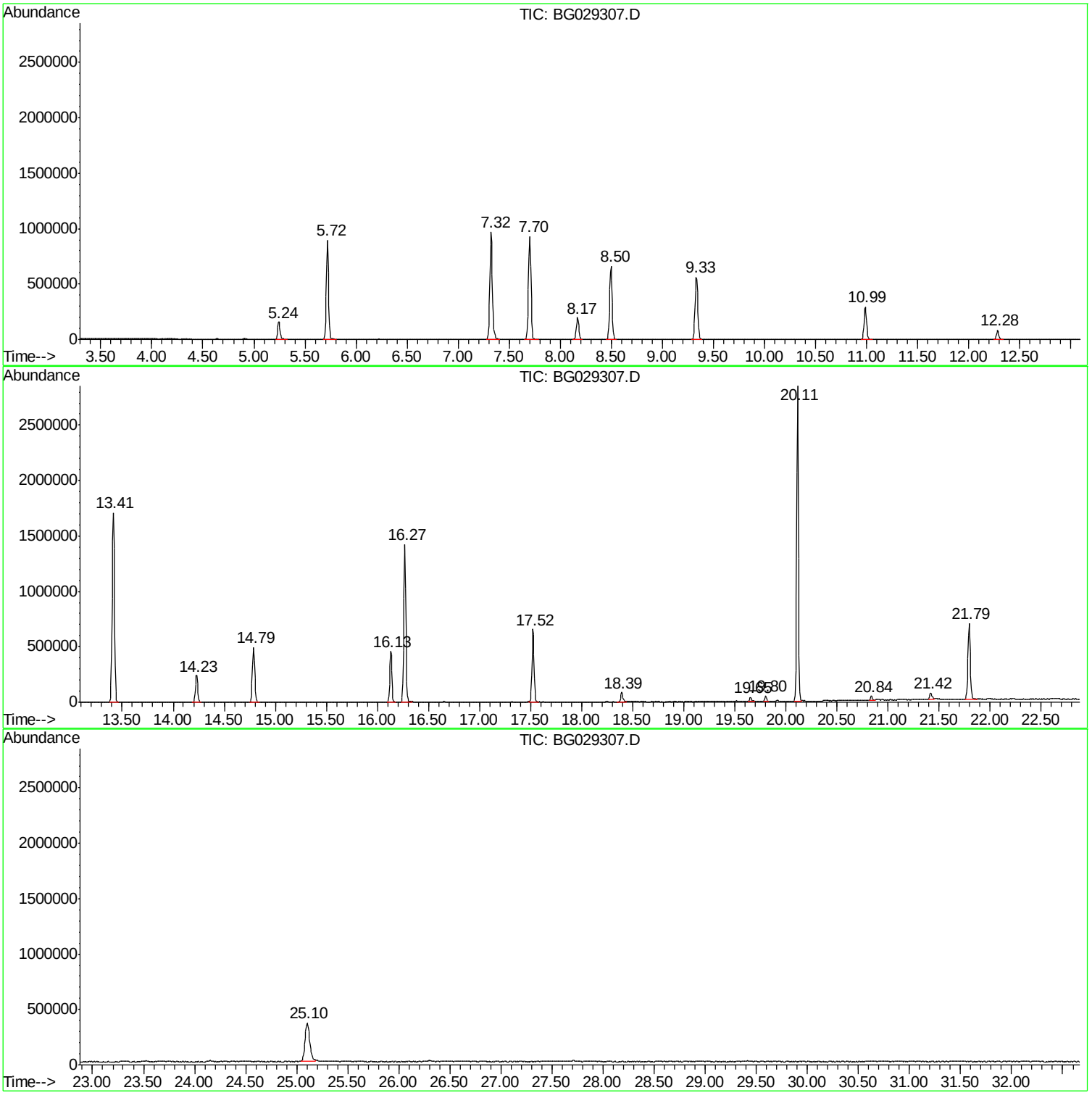
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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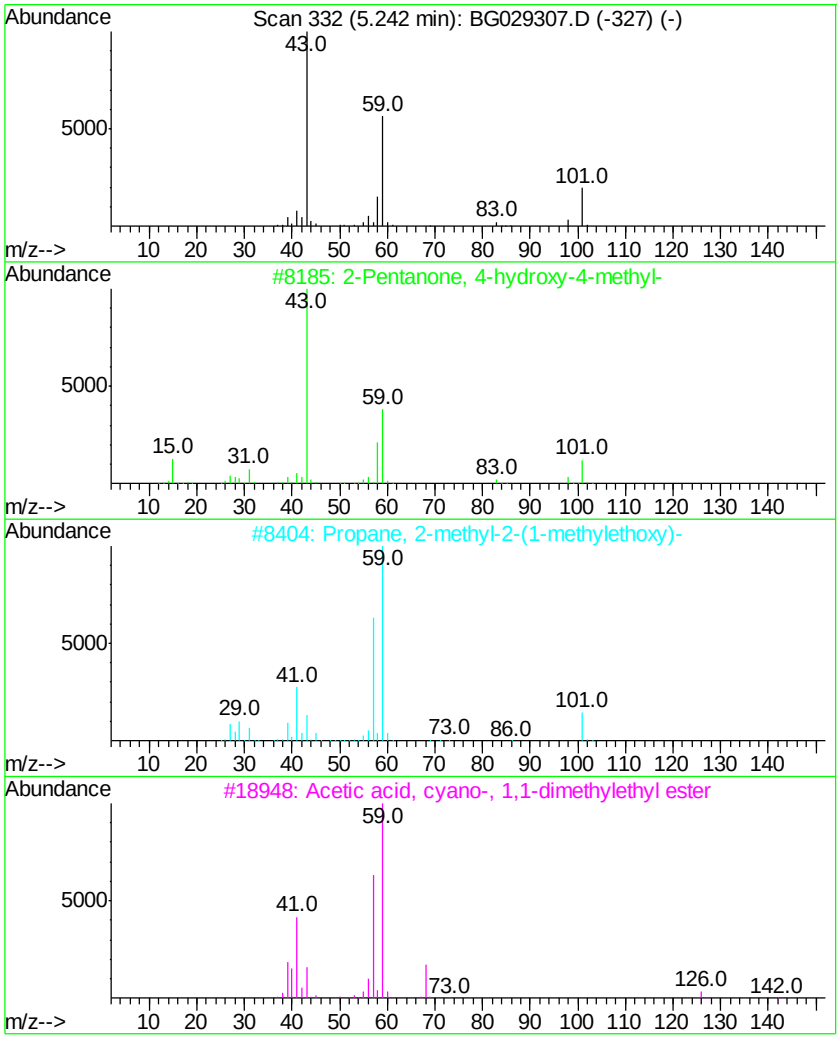
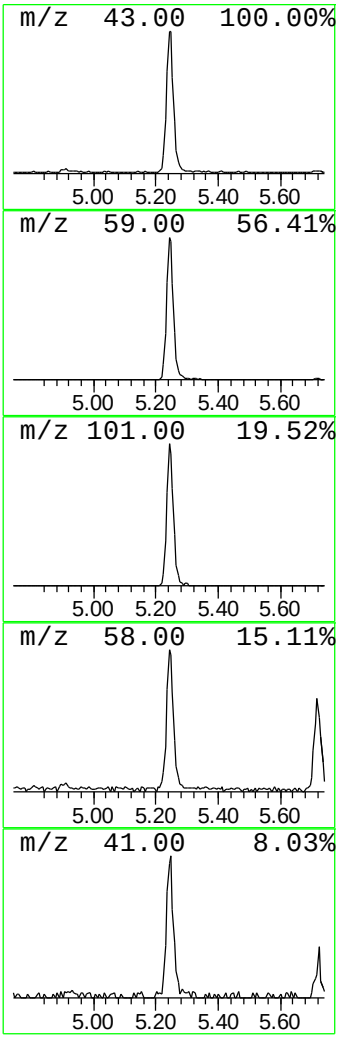
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	15.17 ng	249672	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	45
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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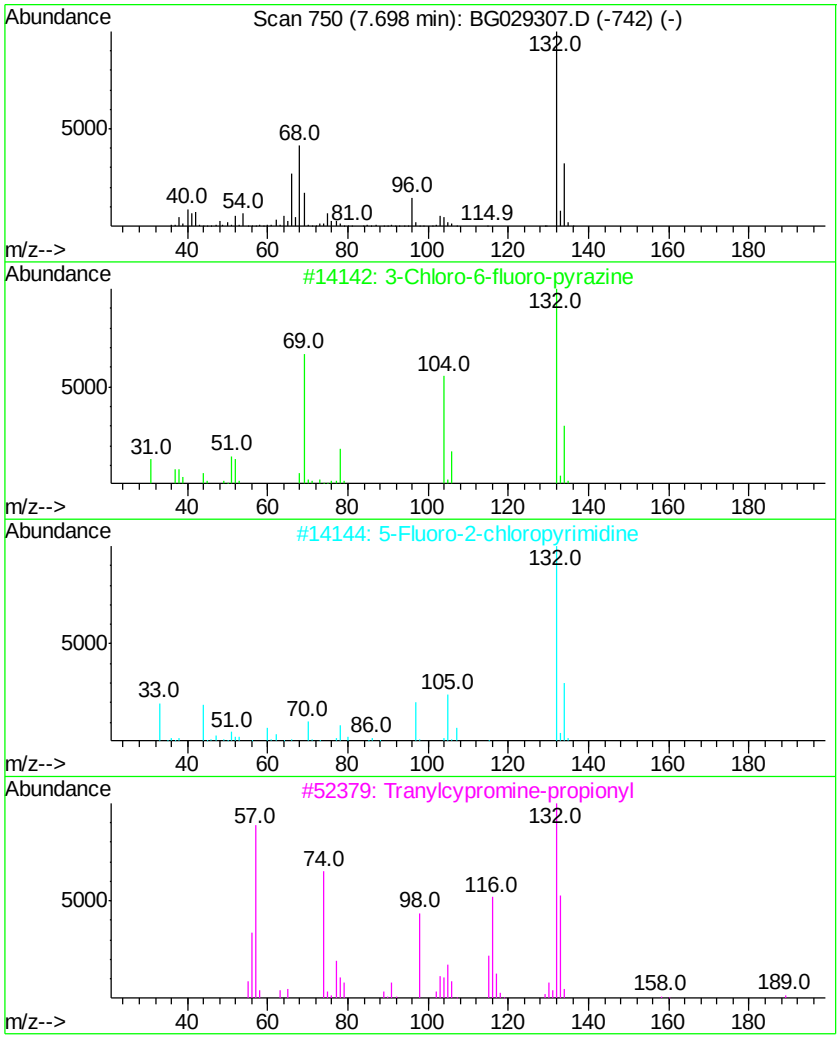
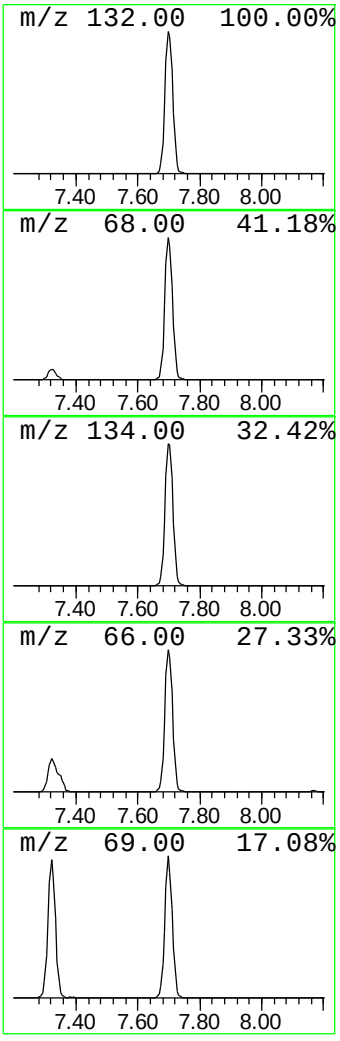
Peak Number 2 unknown7.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	98.36 ng	1618250	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	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	5-Aminoindole	132	C8H8N2	005192-03-0	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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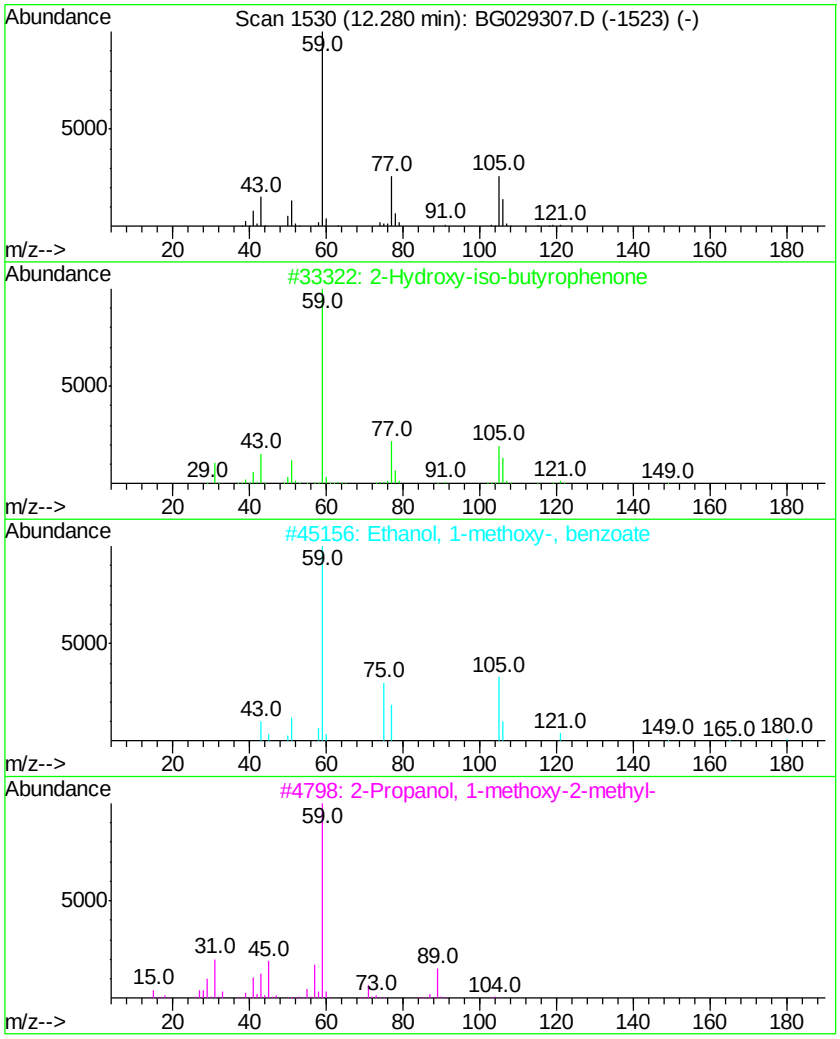
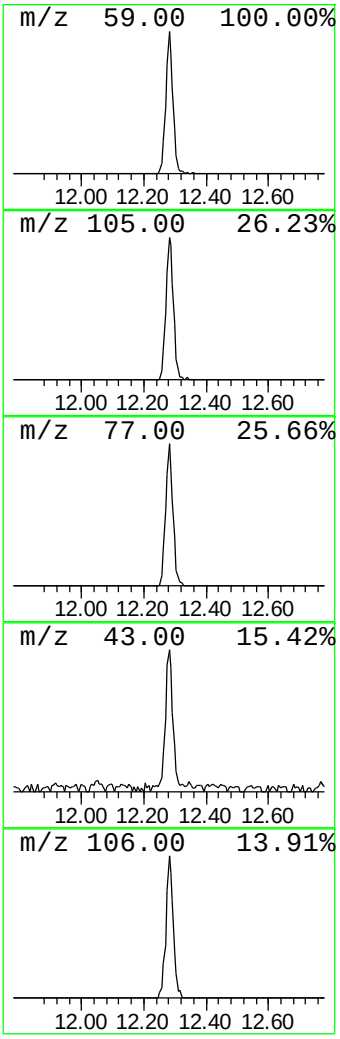
Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.28	5.30 ng	140448	Naphthalene-d8	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	56
3	2-Propanol, 1-methoxy-2-methyl-	104	C5H12O2	003587-64-2	9
4	Ethane, 1,1-dimethoxy-	90	C4H10O2	000534-15-6	9
5	Propionic acid, 2-isopropoxy-, m...	146	C7H14O3	1000151-15-1	9





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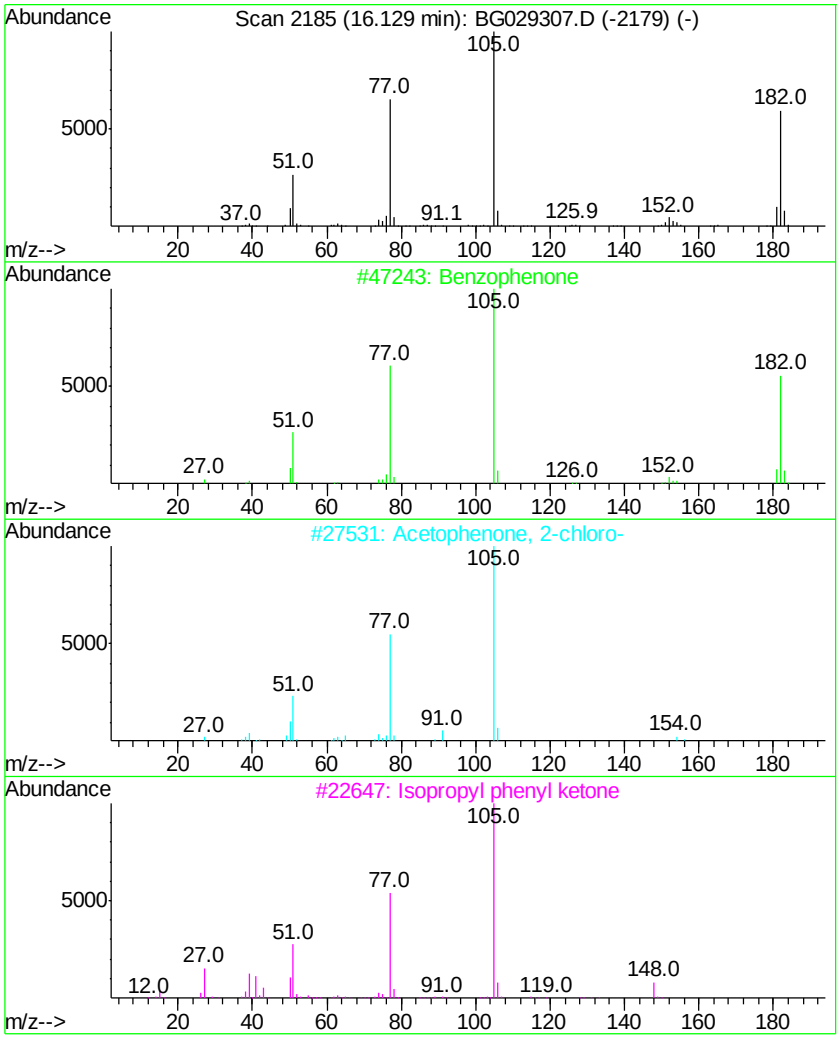
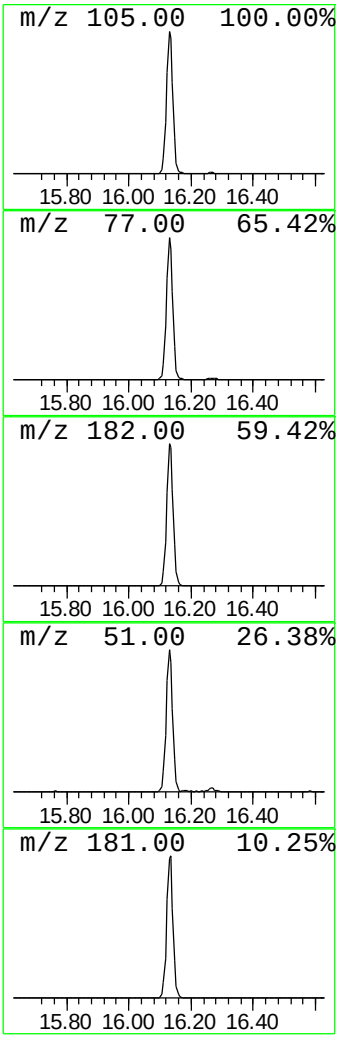
Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	16.47 ng	661962	Acenaphthene-d10	14.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3	Isopropyl phenyl ketone	148	C10H12O	000611-70-1	47
4	Ethanone, 2,2,2-trifluoro-1-phenyl-	174	C8H5F3O	000434-45-7	47
5	Phenacyl thiocyanate	177	C9H7NOS	005399-30-4	47





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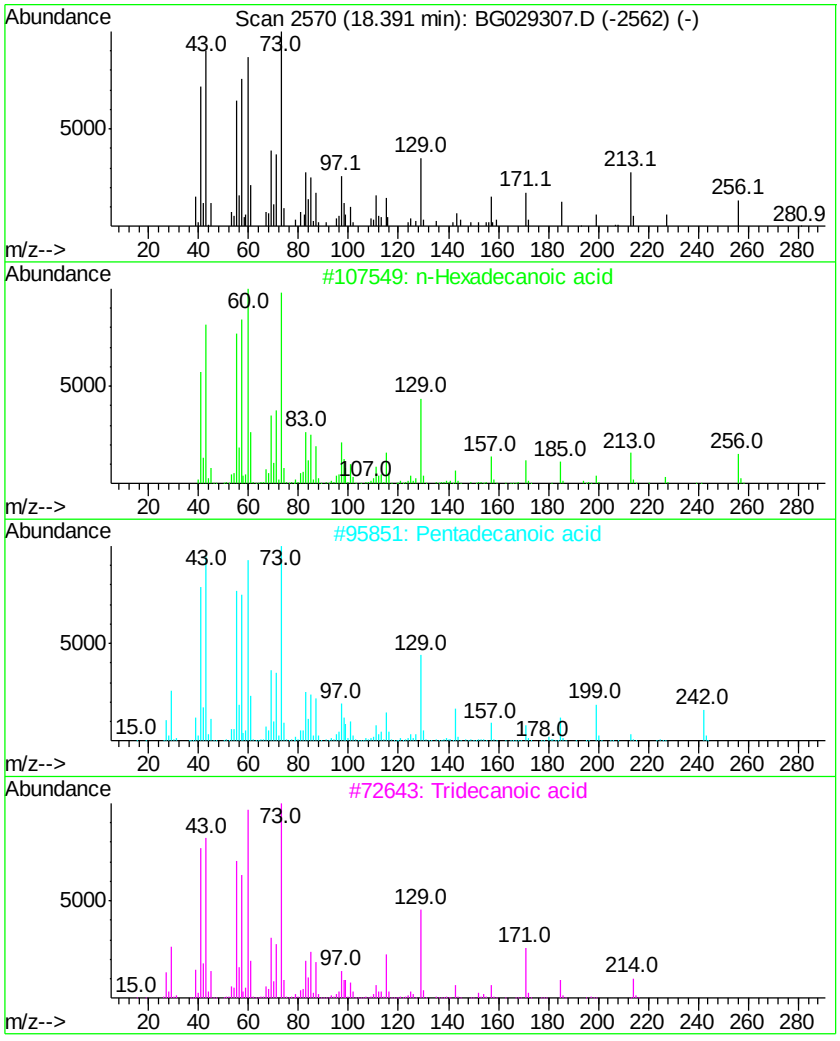
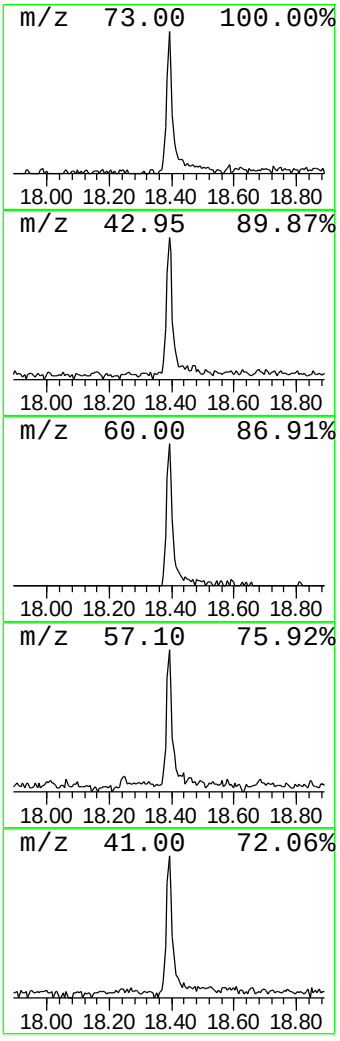
Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.39	2.44 ng	121843	Phenanthrene-d10	17.52

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	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53





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...	5.24	15.2	ng	249672	1	8.17	329060	20.0
unknown7.70	7.70	98.4	ng	1618250	1	8.17	329060	20.0
2-Hydroxy-iso-but...	12.28	5.3	ng	140448	2	10.99	529896	20.0
Benzophenone	16.13	16.5	ng	661962	3	14.79	803649	20.0
n-Hexadecanoic acid	18.39	2.4	ng	121843	4	17.52	997939	20.0