LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG092217\
Data File : BG028887.D
Acq On : 22 Sep 2017 23:19
Operator : SJ/JU
Sample : I5301-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170606-COMP-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:\HPCHEM1\BNA_G\METHODS\8270-BG091217.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	5.382	299	305	310	rBV	27938	47792	1.18%	0.326%
2	5.846	377	384	393	rBV	287239	480695	11.88%	3.280%
3	7.432	646	654	665	rBV	211507	395568	9.78%	2.699%
4	7.808	709	718	732	rBV	457980	827318	20.45%	5.645%
5	8.278	788	798	805	rBV	89385	156329	3.86%	1.067%
6	8.602	843	853	862	rBV	415616	739378	18.27%	5.045%
7	9.448	989	997	1008	rBV	337090	644471	15.93%	4.398%
8	11.093	1270	1277	1288	rBV	111566	221500	5.47%	1.511%
9	13.513	1680	1689	1700	rBV	1105062	1695138	41.89%	11.567%
10	14.401	1835	1840	1846	rVB2	26965	40890	1.01%	0.279%
11	14.894	1917	1924	1931	rBV2	223115	366503	9.06%	2.501%
12	15.276	1982	1989	1995	rBV	72836	107294	2.65%	0.732%
13	15.658	2049	2054	2058	rBV	158739	200488	4.95%	1.368%
14	16.387	2169	2178	2191	rBV	1176352	1904352	47.06%	12.995%
15	17.644	2385	2392	2403	rBV	396925	618820	15.29%	4.223%
16	18.284	2493	2501	2507	rBV3	134497	187545	4.63%	1.280%
17	19.888	2766	2774	2782	rBV	293536	351271	8.68%	2.397%
18	20.229	2826	2832	2839	rBV	2982784	4046360	100.00%	27.612%
19	21.962	3120	3127	3138	rBV	445863	798253	19.73%	5.447%
20	23.161	3326	3331	3341	rBV	24201	51112	1.26%	0.349%
21	25.411	3702	3714	3727	rVB2	244463	773447	19.11%	5.278%

Sum of corrected areas: 14654524

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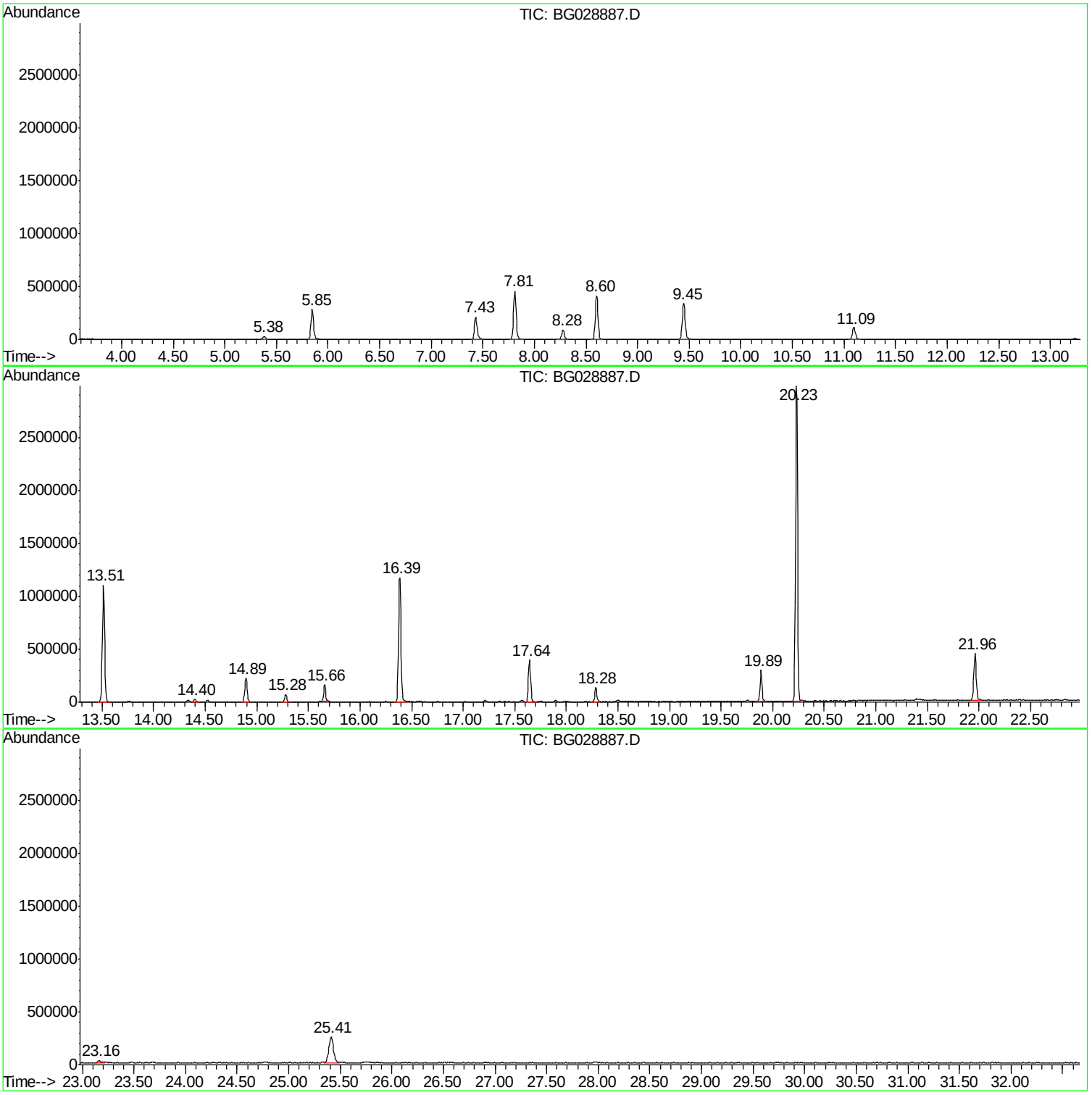
BNA_G
ClientSampleId :
20170606-COMP-C

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.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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TIC Library : C:\Database\NIST11.L
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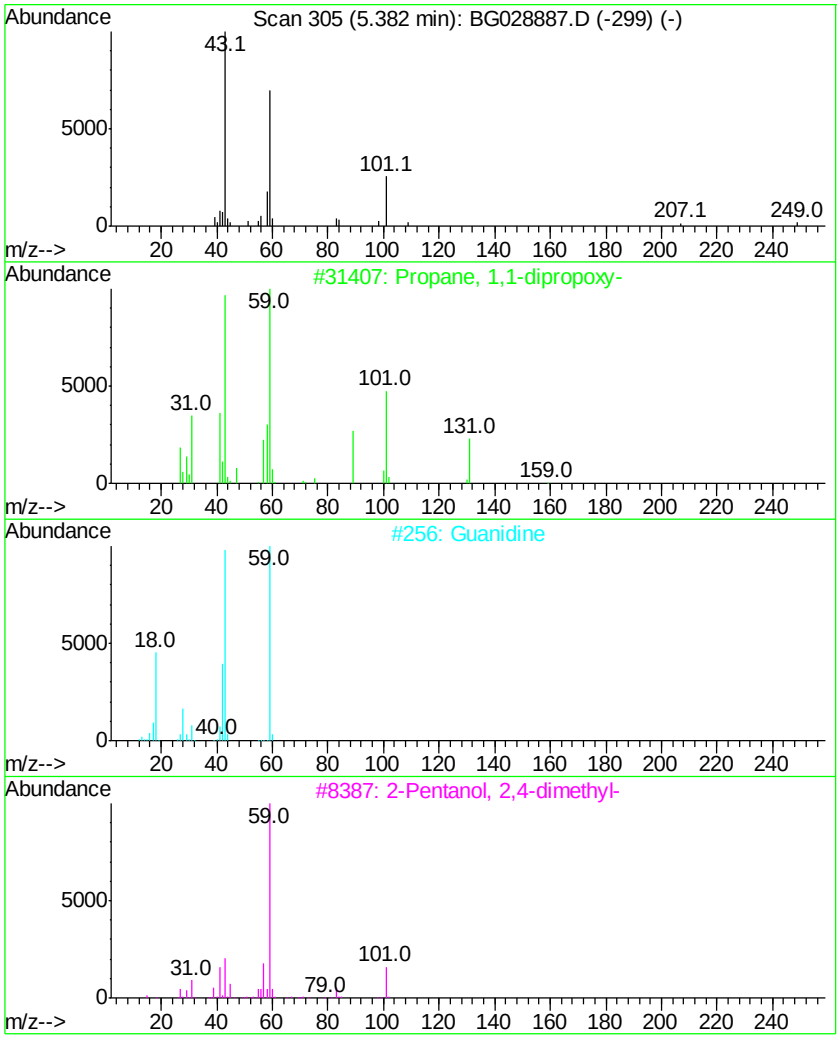
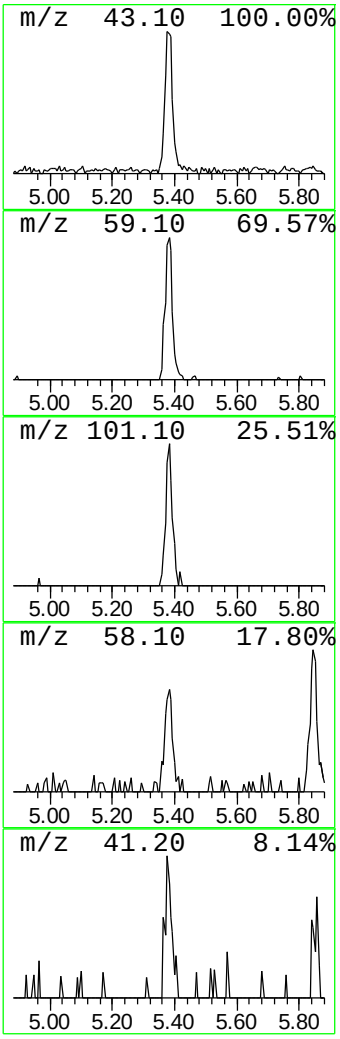
****

Peak Number 1 Propane, 1,1-dipropoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.38	6.11 ng	47792	1,4-Dichlorobenzene-d4	8.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	50
2	Guanidine	59	CH5N3	000113-00-8	47
3	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	42
4	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	12





Library Search Compound Report

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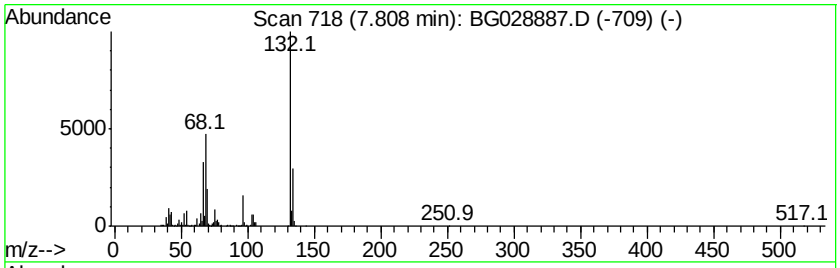
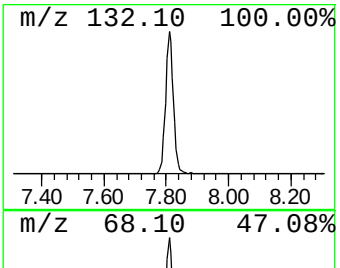
****

Peak Number 2 unknown7.81 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.81	105.84 ng	827318	1,4-Dichlorobenzene-d4	8.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





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Instrument : BNA_G
ClientSampleId : 20170606-COMP-C

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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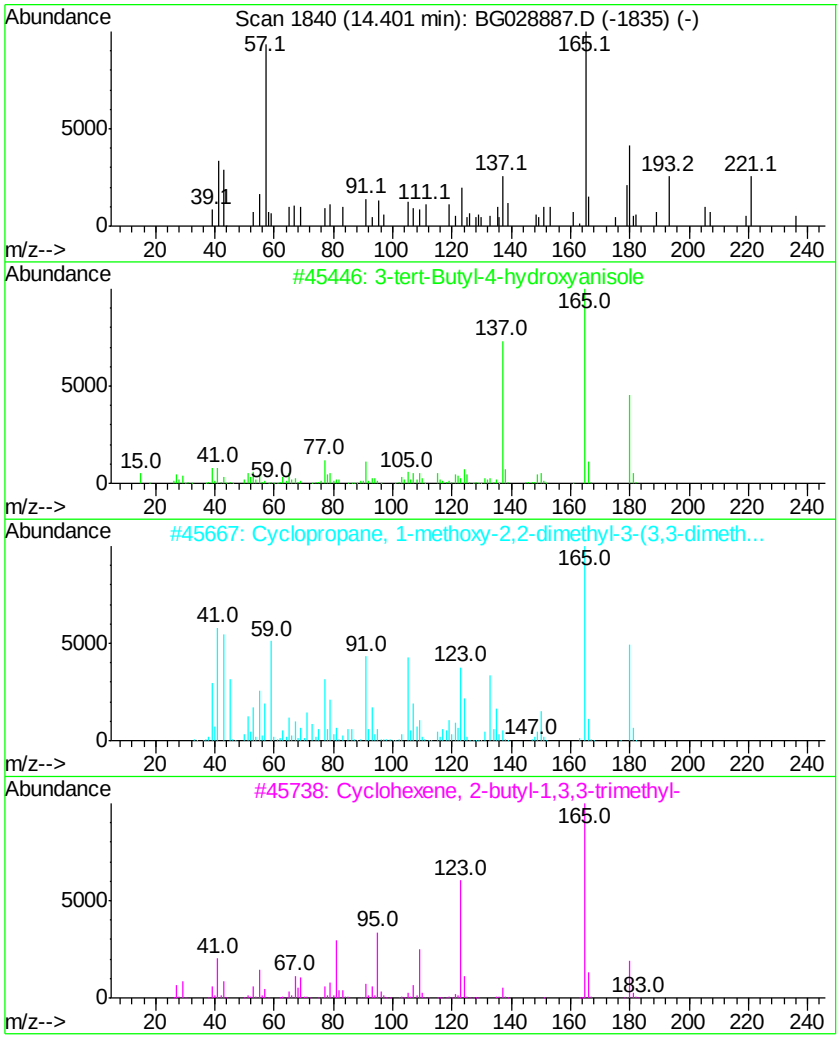
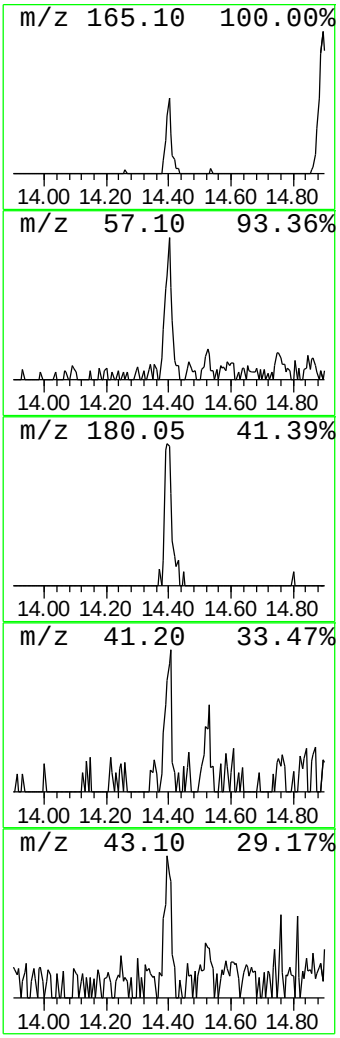
****

Peak Number 4 3-tert-Butyl-4-hydroxyanisole Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.40	2.23 ng	40890	Acenaphthene-d10	14.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	50
2	Cyclopropane, 1-methoxy-2,2-dime...	180	C12H20O	1000271-82-9	49
3	Cyclohexene, 2-butyl-1,3,3-trime...	180	C13H24	003293-50-3	49
4	Thiophene, 2-[(trimethylsilyl)et...	180	C9H12SSi	040231-03-6	46
5	Ethanone, 1-(3,4-dimethoxyphenyl)-	180	C10H12O3	001131-62-0	46





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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170606-COMP-C

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
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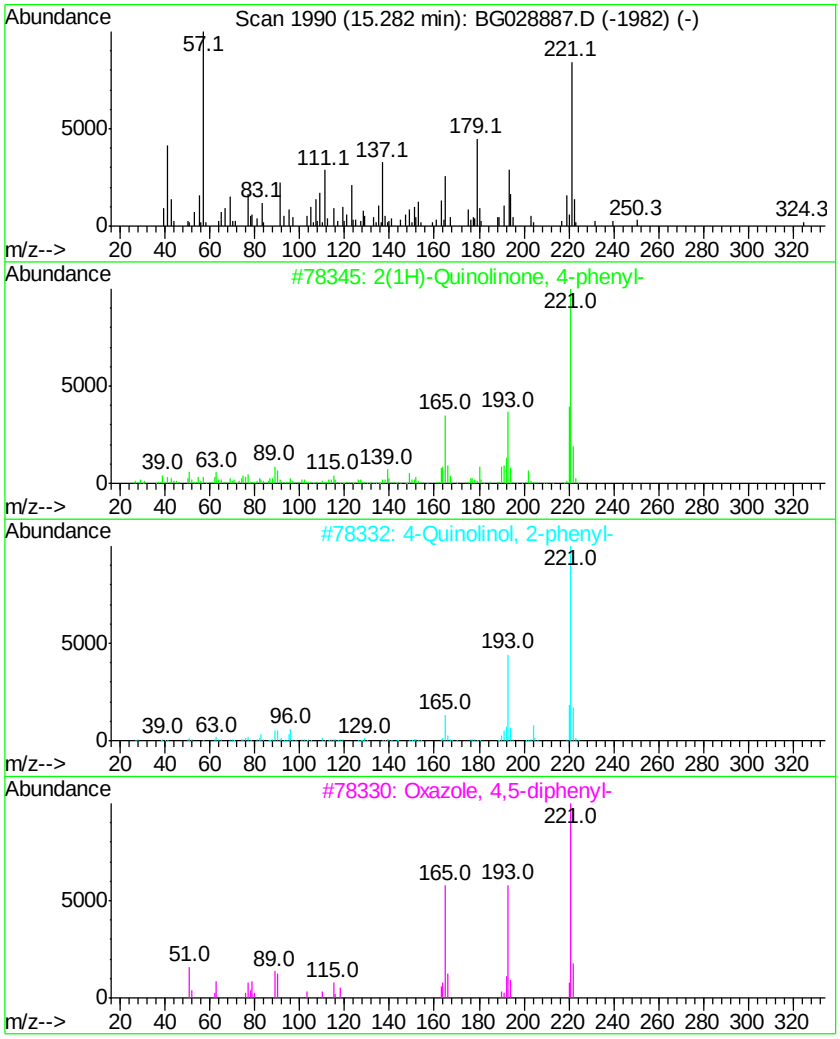
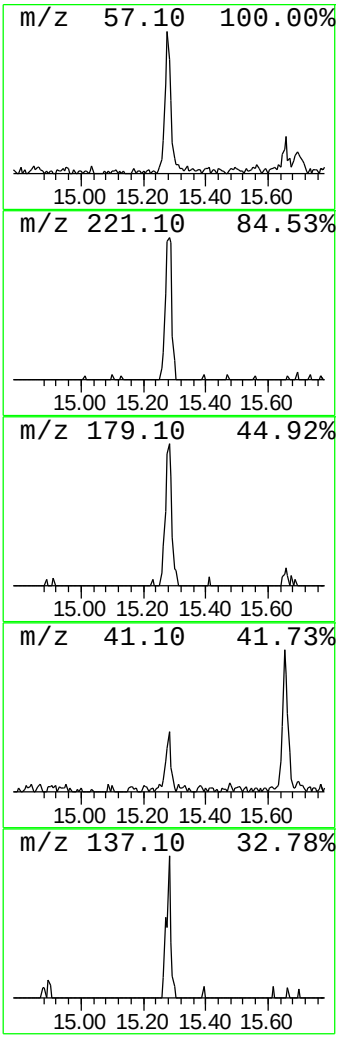
****

Peak Number 5 2(1H)-Quinolinone, 4-phenyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.28	5.86 ng	107294	Acenaphthene-d10	14.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Quinolinone, 4-phenyl-	221	C15H11NO	005855-57-2	53
2	4-Quinolinol, 2-phenyl-	221	C15H11NO	001144-20-3	38
3	Oxazole, 4,5-diphenyl-	221	C15H11NO	004675-18-7	37
4	Oxazole, 2,5-diphenyl-	221	C15H11NO	000092-71-7	35
5	1H-1,2,4-Triazole, 3,5-diphenyl-	221	C14H11N3	002039-06-7	30





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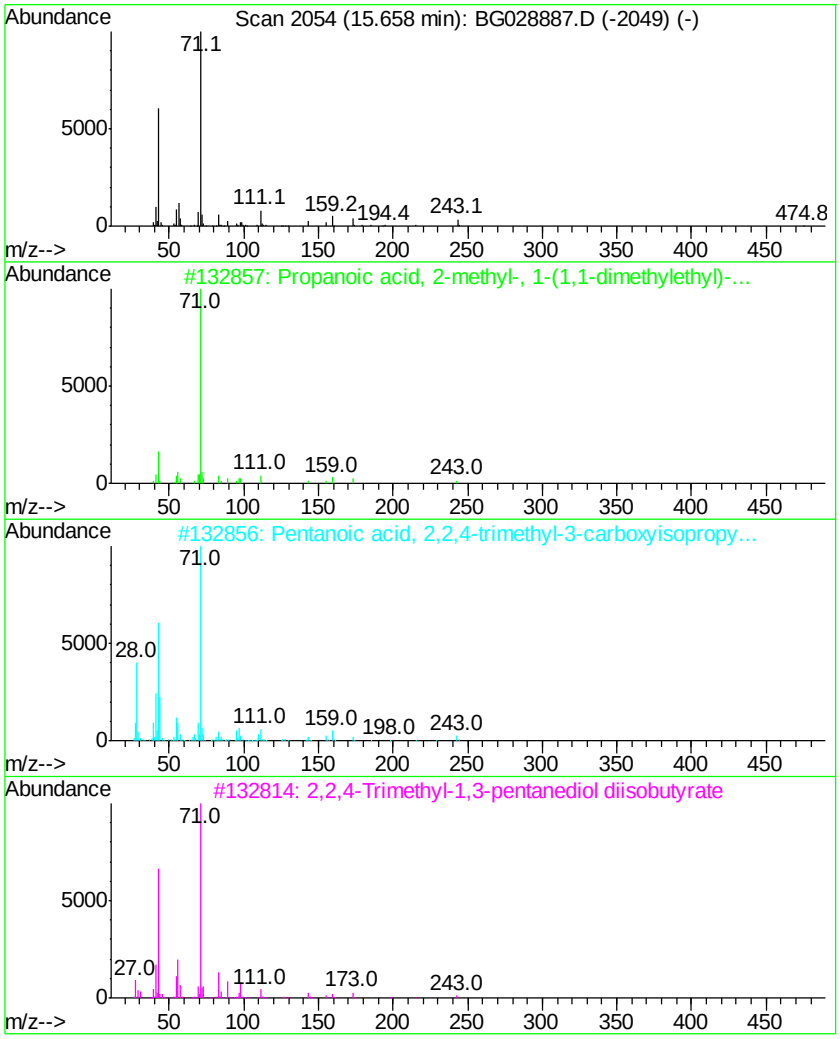
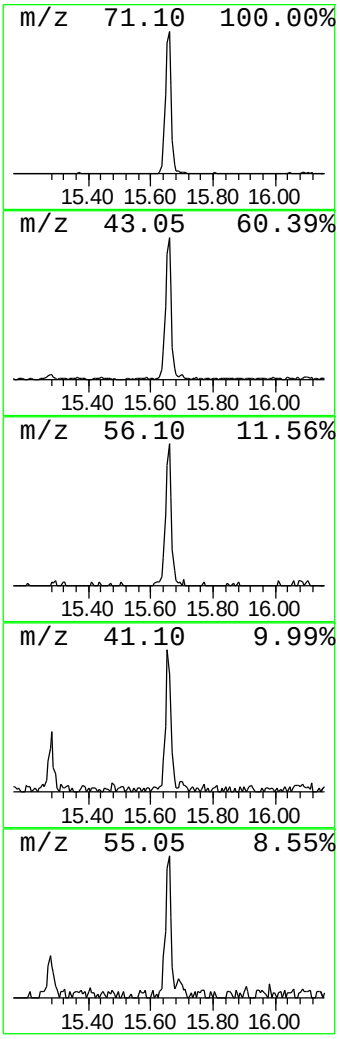
****

Peak Number 6 Propanoic acid, 2-methyl-, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.66	10.94 ng	200488	Acenaphthene-d10	14.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-(1,...	286	C16H30O4	074381-40-1	72
2	Pentanoic acid, 2,2,4-trimethyl-...	286	C16H30O4	1000140-77-5	64
3	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	56
4	Fumaric acid, nonyl tetrahydrofu...	326	C18H30O5	1000330-58-3	53
5	Butyric acid, 3-tridecyl ester	270	C17H34O2	1000280-56-8	50





Library Search Compound Report

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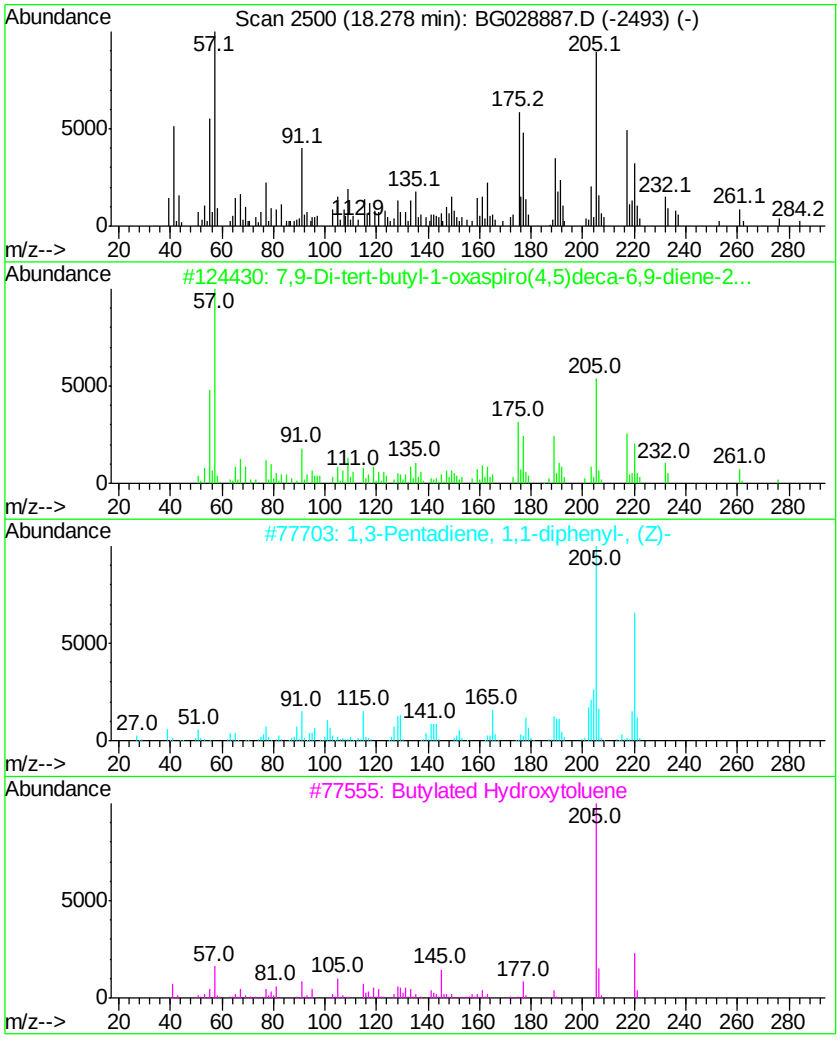
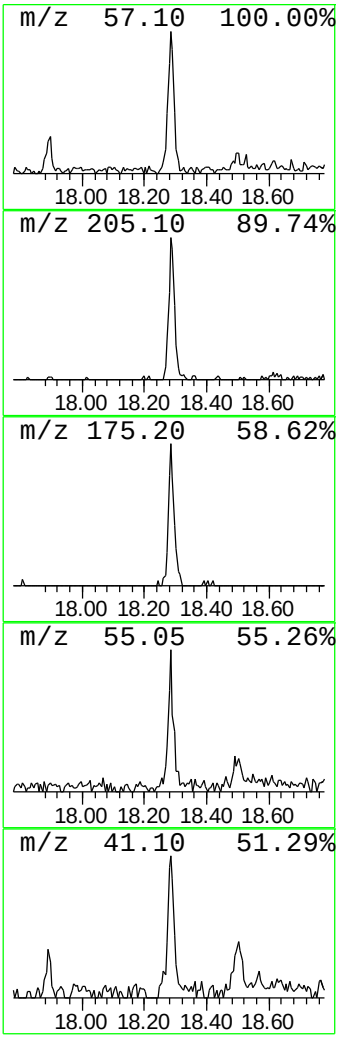
****

Peak Number 7 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.28	6.06 ng	187545	Phenanthrene-d10	17.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	94
2	1,3-Pentadiene, 1,1-diphenyl-, (Z)-	220	C17H16	015295-31-5	49
3	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	38
4	2H-1-Benzopyran, 6,7-dimethoxy-2...	220	C13H16O3	000644-06-4	30
5	2,5-Cyclohexadien-1-one, 2,6-bis...	232	C16H24O	006738-27-8	30





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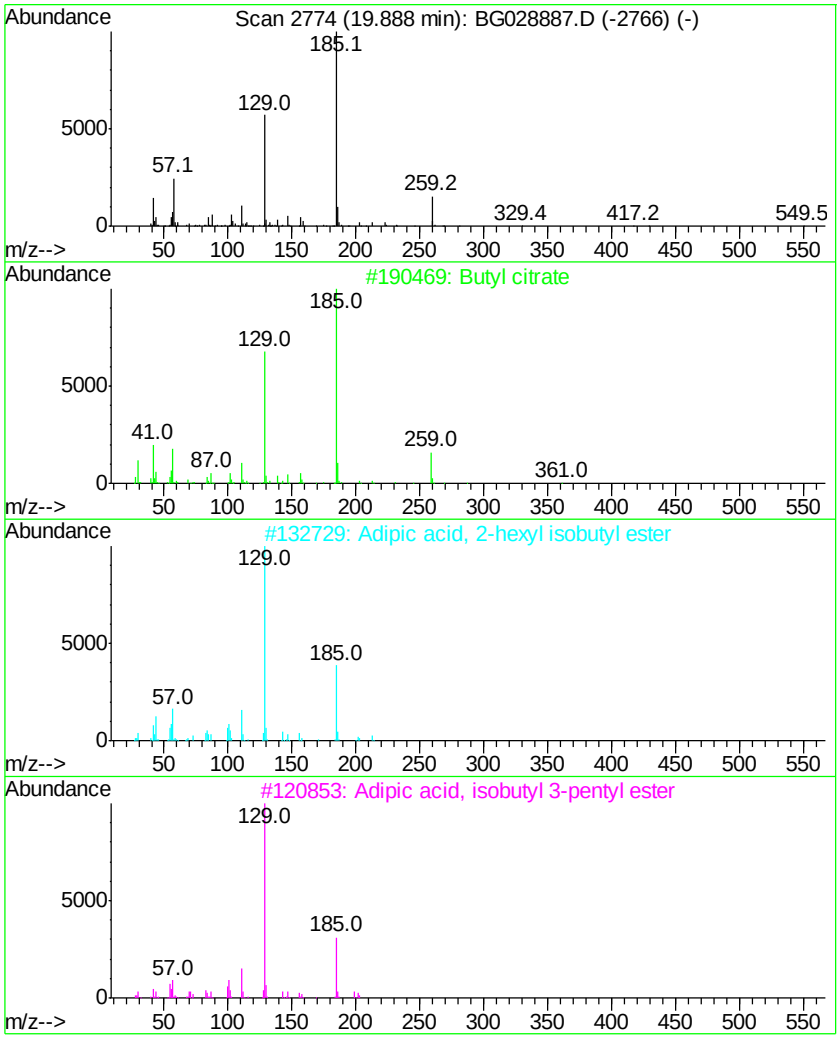
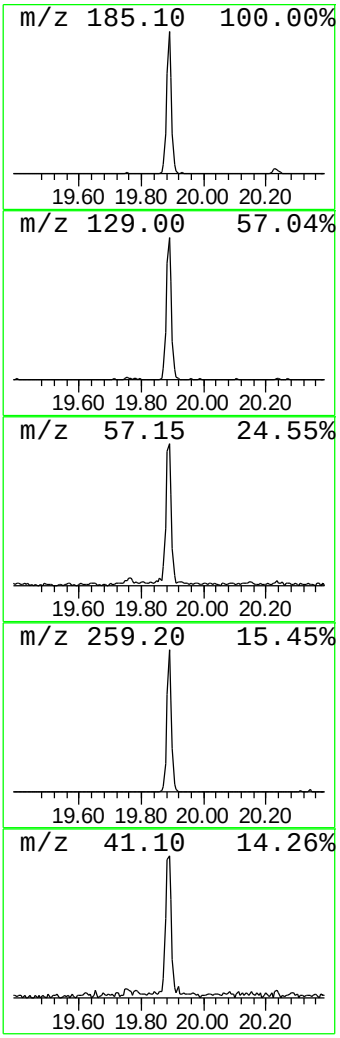
****

Peak Number 8 Butyl citrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.89	8.80 ng	351271	Chrysene-d12	21.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl citrate	360	C18H32O7	000077-94-1	91
2	Adipic acid, 2-hexyl isobutyl ester	286	C16H30O4	1000353-70-9	56
3	Adipic acid, isobutyl 3-pentyl e...	272	C15H28O4	1000324-60-4	56
4	Hexanedioic acid, bis(2-methylpr...	258	C14H26O4	000141-04-8	56
5	Adipic acid, butyl 2-decyl ester	342	C20H38O4	1000353-59-7	50





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 1,1-dipr...	5.38	6.1	ng	47792	1	8.28	156329	20.0
unknown7.81	7.81	105.8	ng	827318	1	8.28	156329	20.0
3-tert-Butyl-4-hy...	14.40	2.2	ng	40890	3	14.89	366503	20.0
2(1H)-Quinolinone...	15.28	5.9	ng	107294	3	14.89	366503	20.0
Propanoic acid, 2...	15.66	10.9	ng	200488	3	14.89	366503	20.0
7,9-Di-tert-butyl...	18.28	6.1	ng	187545	4	17.64	618820	20.0
Butyl citrate	19.89	8.8	ng	351271	5	21.96	798253	20.0