LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG090418\
Data File : BG036529.D
Acq On : 4 Sep 2018 13:16
Operator : JU/SJ
Sample : J4712-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-03

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-BG082318.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	5.165	313	319	326	rVB	42188	65235	1.87%	0.293%
2	5.629	390	398	410	rVB	983828	1606876	46.16%	7.223%
3	7.210	659	667	679	rBV	1039113	1836093	52.74%	8.254%
4	7.592	724	732	740	rBV	959492	1657262	47.61%	7.450%
5	8.056	805	811	818	rBV	235349	400230	11.50%	1.799%
6	8.379	858	866	875	rBV	696155	1216906	34.96%	5.470%
7	9.219	1000	1009	1017	rBV	606488	1063907	30.56%	4.783%
8	10.864	1278	1289	1299	rBV	327503	586673	16.85%	2.637%
9	13.309	1696	1705	1715	rBV	1526855	2363755	67.90%	10.626%
10	14.125	1839	1844	1850	rBV	161131	234339	6.73%	1.053%
11	14.684	1928	1939	1948	rBV2	513735	839609	24.12%	3.774%
12	16.164	2184	2191	2202	rBV	1250806	1972122	56.65%	8.865%
13	17.427	2399	2406	2413	rBV	726489	1099738	31.59%	4.944%
14	18.309	2549	2556	2565	rBV	95431	146366	4.20%	0.658%
15	19.731	2793	2798	2803	rVB	210090	243043	6.98%	1.093%
16	19.842	2814	2817	2821	rVB2	33051	39014	1.12%	0.175%
17	20.030	2843	2849	2861	rBV	2581802	3481277	100.00%	15.649%
18	20.770	2970	2975	2979	rVB	167536	189042	5.43%	0.850%
19	21.346	3068	3073	3090	rBV3	82077	280524	8.06%	1.261%
20	21.687	3124	3131	3144	rBV	760328	1284154	36.89%	5.773%
21	21.893	3162	3166	3172	rVB	32445	48114	1.38%	0.216%
22	22.498	3265	3269	3275	rBV2	27833	46839	1.35%	0.211%
23	23.197	3382	3388	3394	rVB2	36486	68062	1.96%	0.306%
24	23.385	3416	3420	3426	rVB3	31524	57328	1.65%	0.258%
25	24.008	3520	3526	3534	rVB2	32535	68315	1.96%	0.307%
26	24.901	3667	3678	3699	rVB2	413247	1293178	37.15%	5.813%
27	26.088	3875	3880	3890	rVB4	21031	57361	1.65%	0.258%

Sum of corrected areas: 22245362

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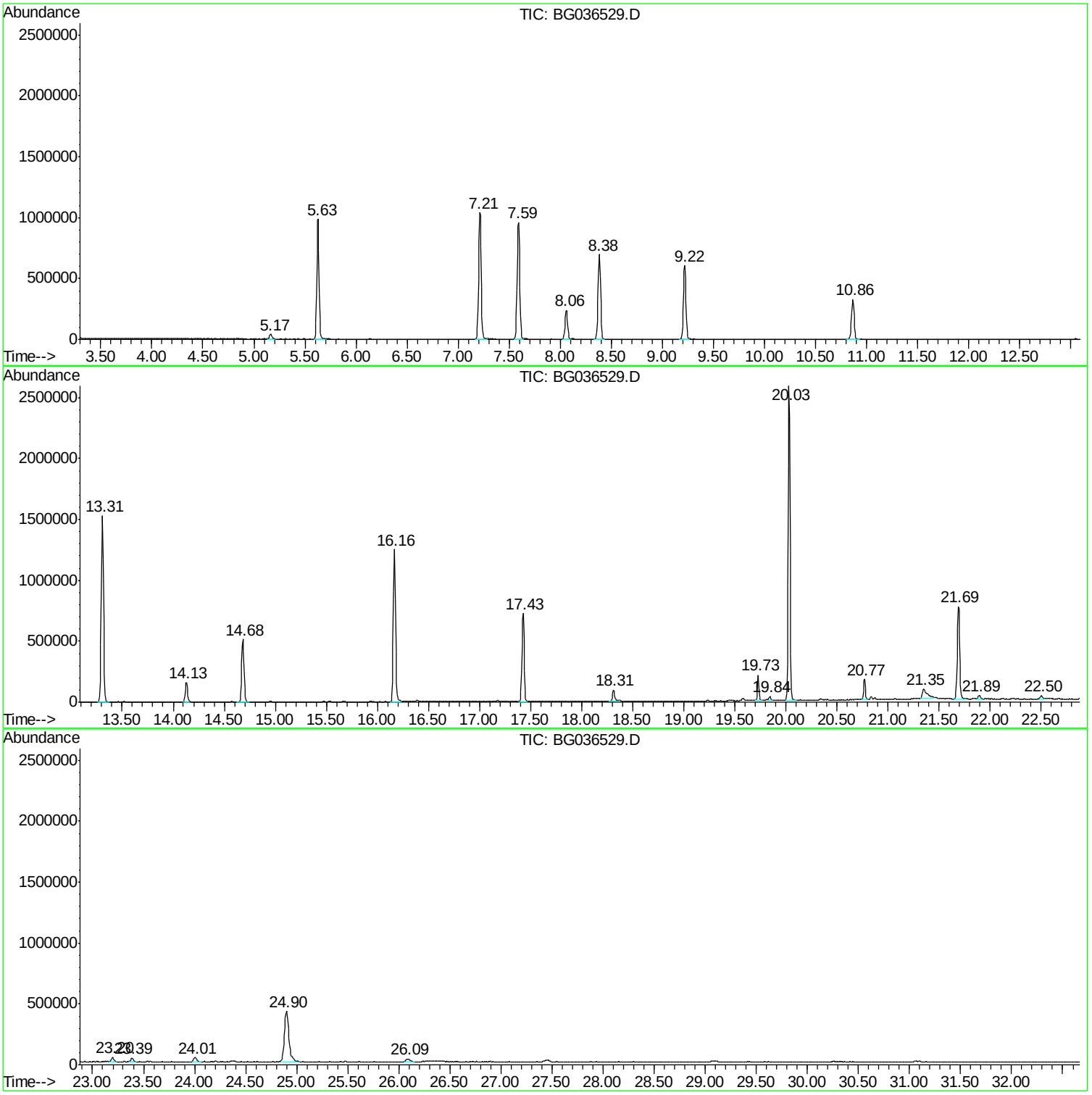
Instrument : BNA_G
ClientSampleId : SB-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.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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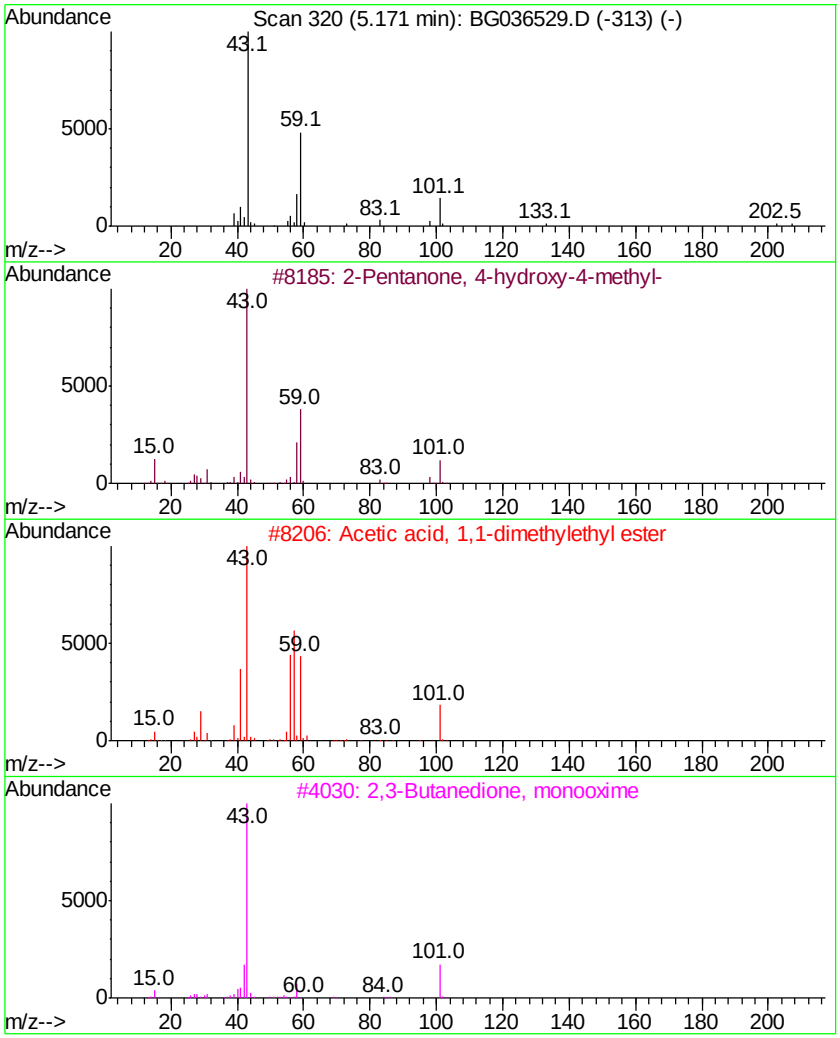
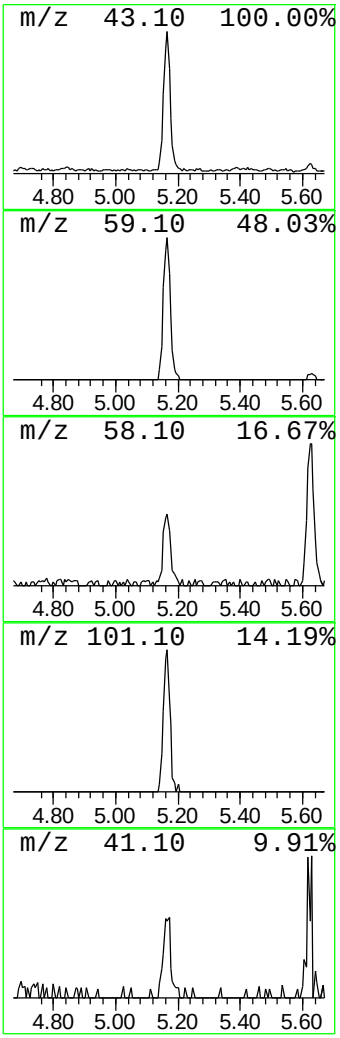
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	3.26 ng	65235	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





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Misc :
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Instrument : BNA_G
ClientSampleId : SB-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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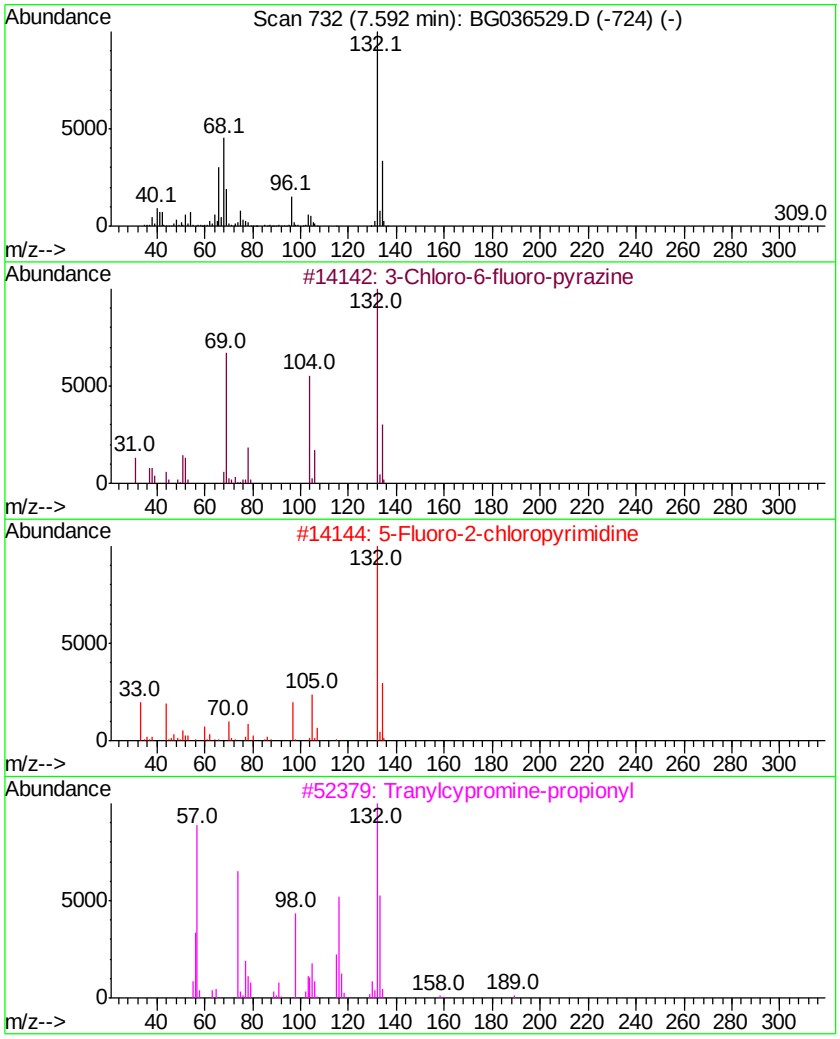
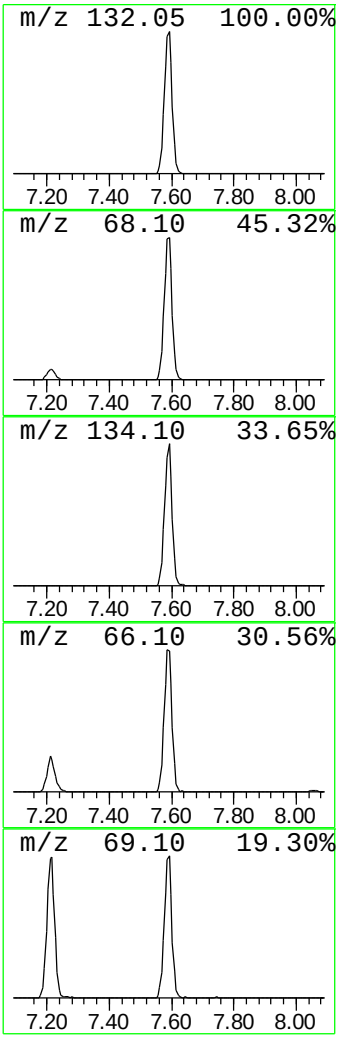
Peak Number 2 unknown7.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	82.82 ng	1657260	1,4-Dichlorobenzene-d4	8.06

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	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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Data File : BG036529.D
Acq On : 4 Sep 2018 13:16
Operator : JU/SJ
Sample : J4712-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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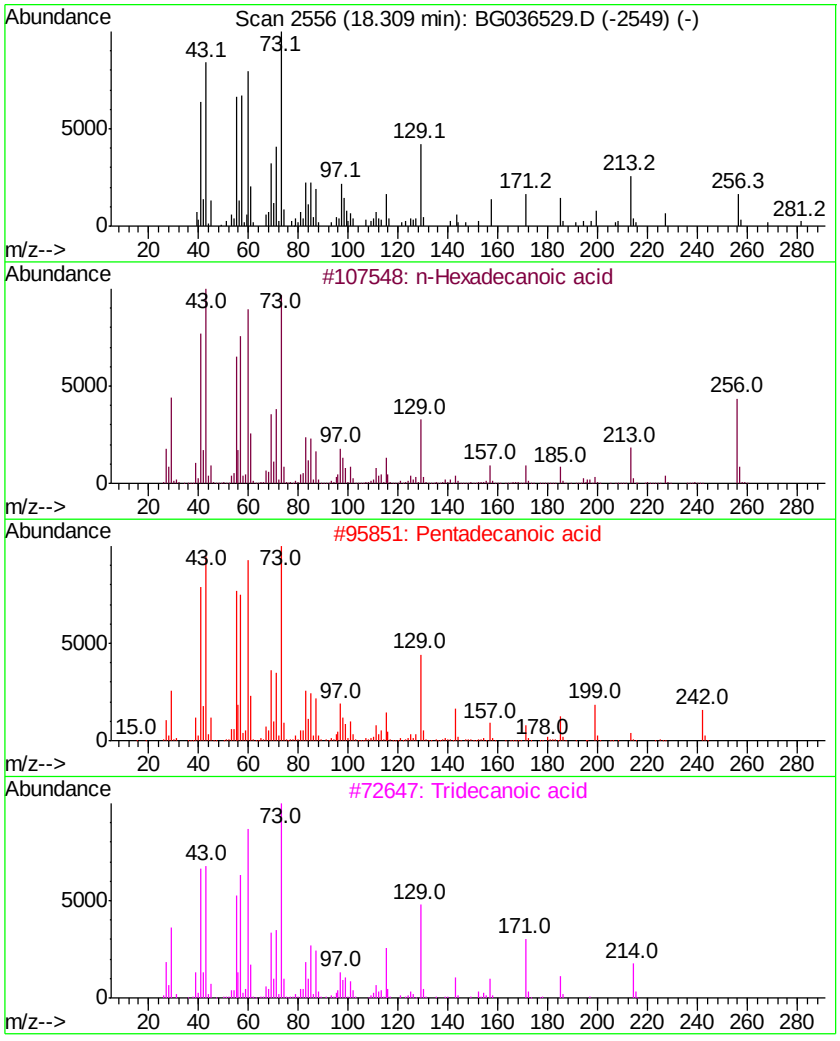
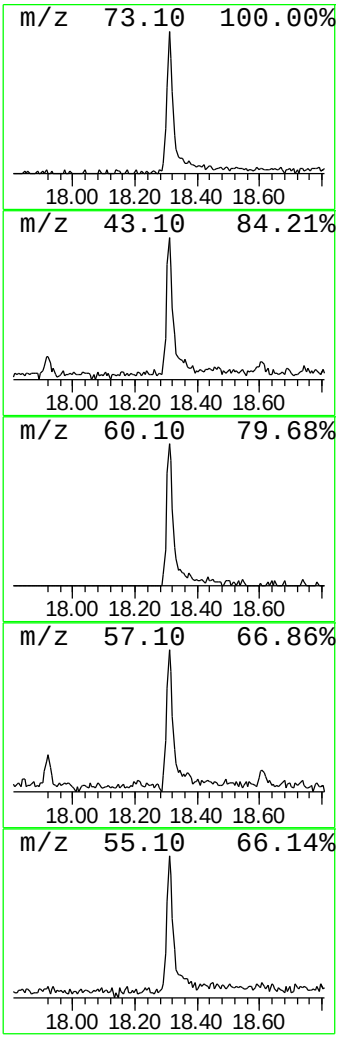
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.31	2.66 ng	146366	Phenanthrene-d10	17.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	70
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	2-Butenoic acid, 2-methoxy-3-met...	144	C7H12O3	056009-32-6	18





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Data File : BG036529.D
Acq On : 4 Sep 2018 13:16
Operator : JU/SJ
Sample : J4712-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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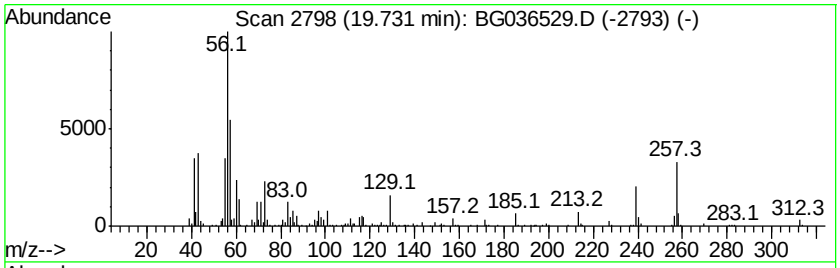
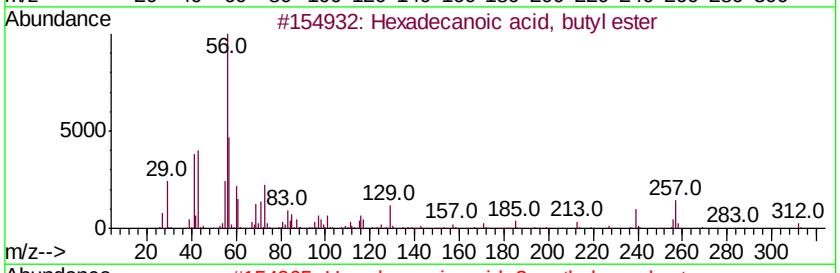
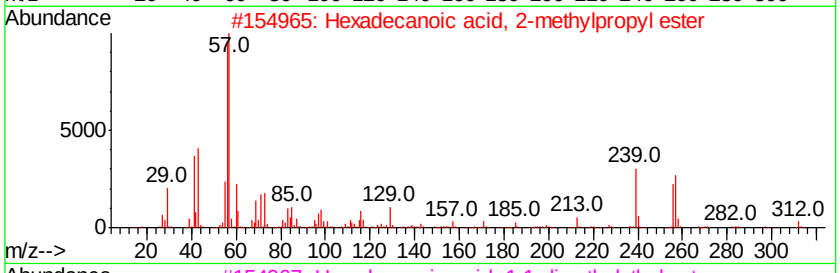
Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 4

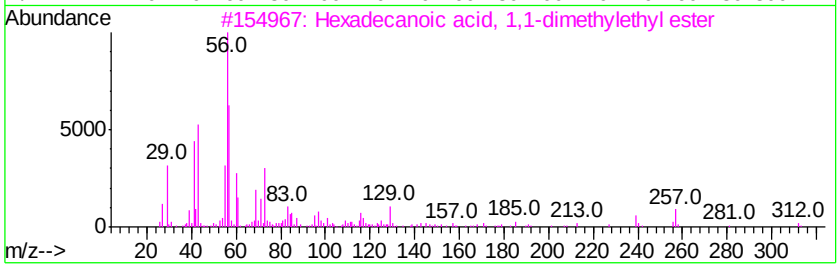
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.73	3.79 ng	243043	Chrysene-d12	21.69

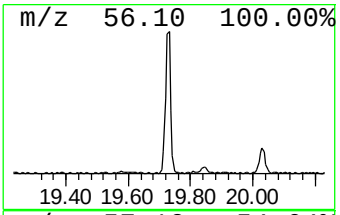
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	98
2	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	81
3	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	46
4	4-Propylcyclohexylamine	141	C9H19N	102653-37-2	30
5	Cyclopentanone, 2,2-dimethyl-	112	C7H12O	004541-32-6	30

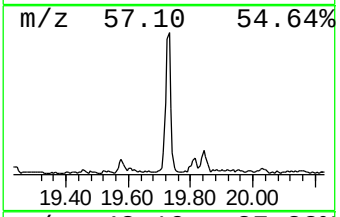


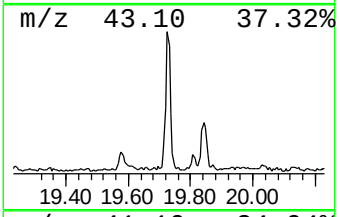


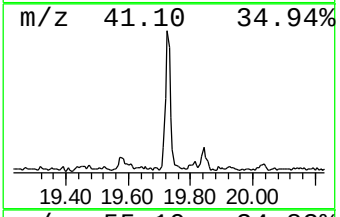


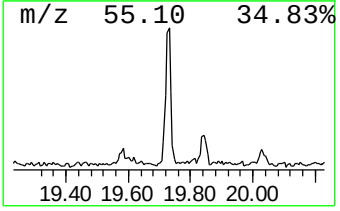












Library Search Compound Report

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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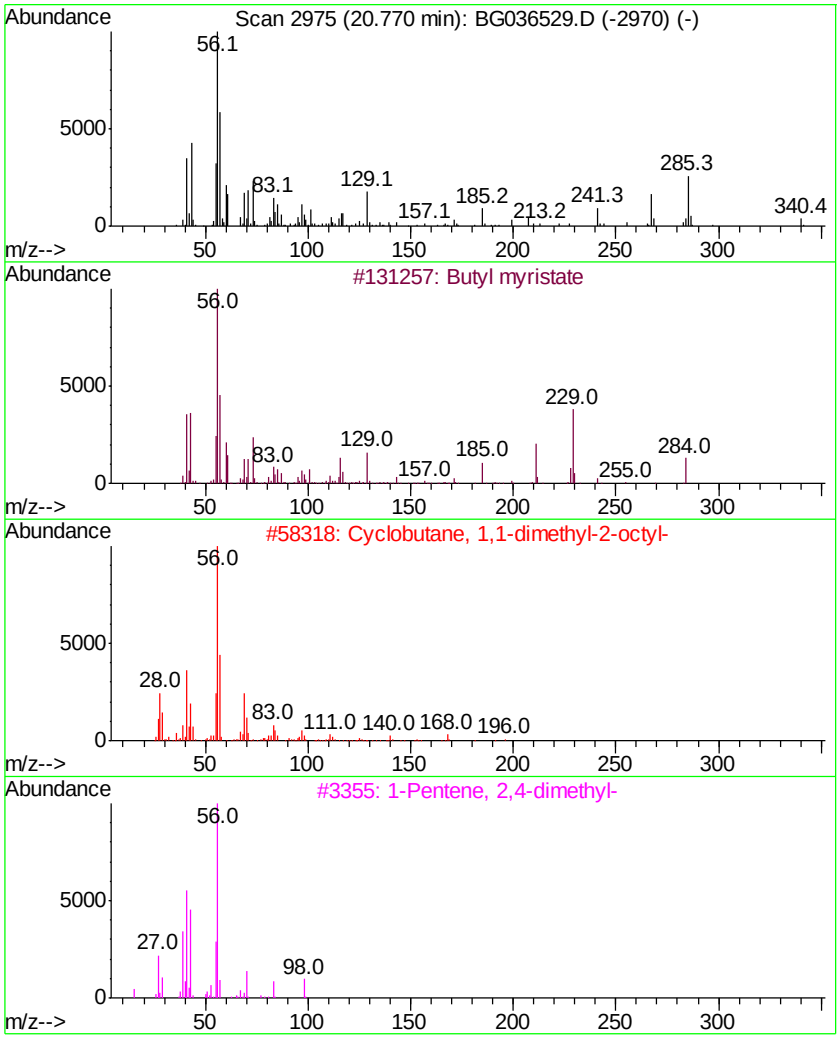
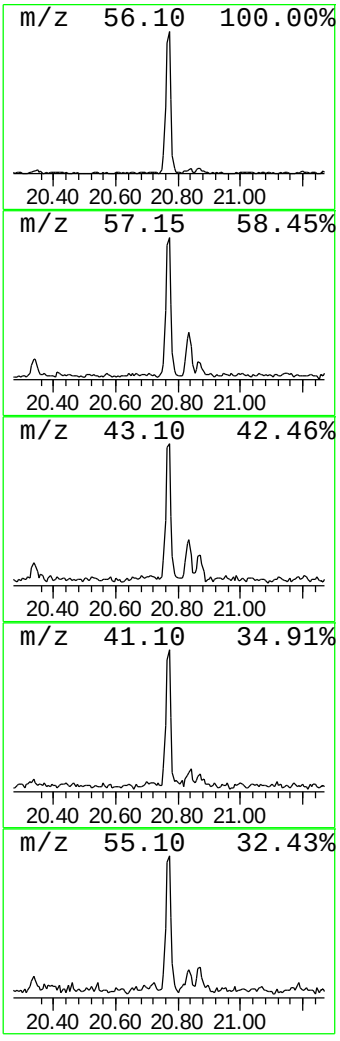
****

Peak Number 6 Butyl myristate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.77	2.94 ng	189042	Chrysene-d12	21.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	58
2	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
3	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	35
4	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	35
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35





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Misc :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

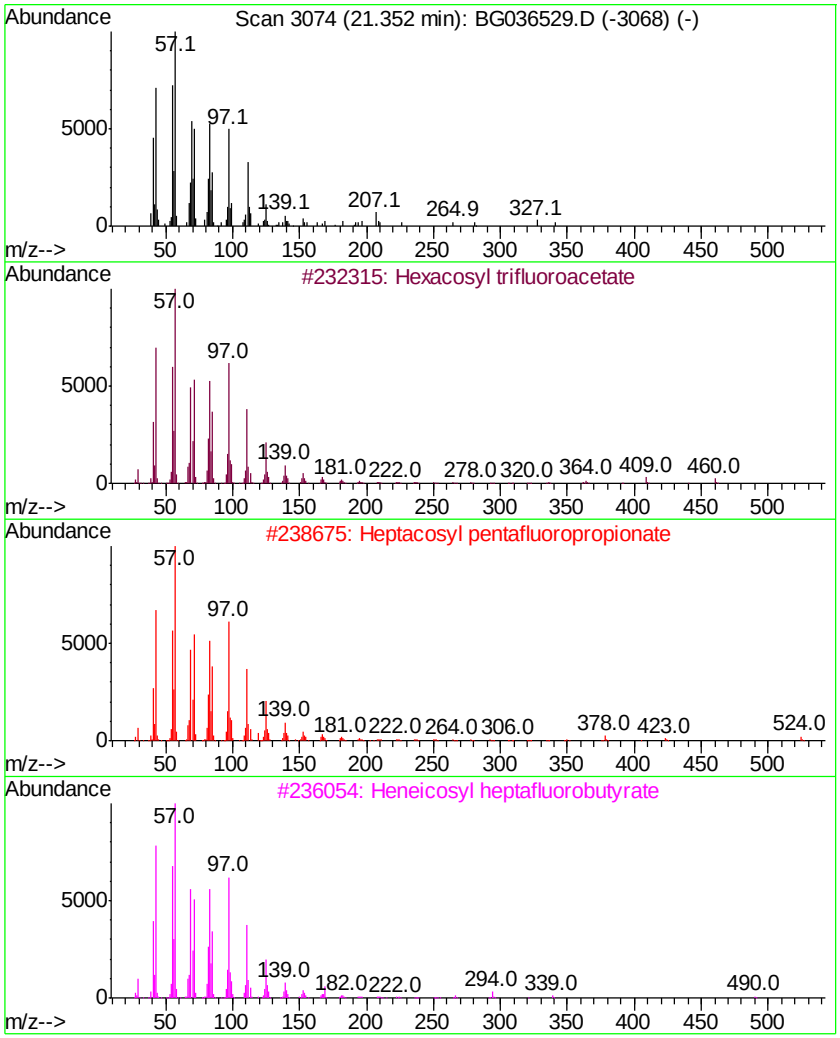
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

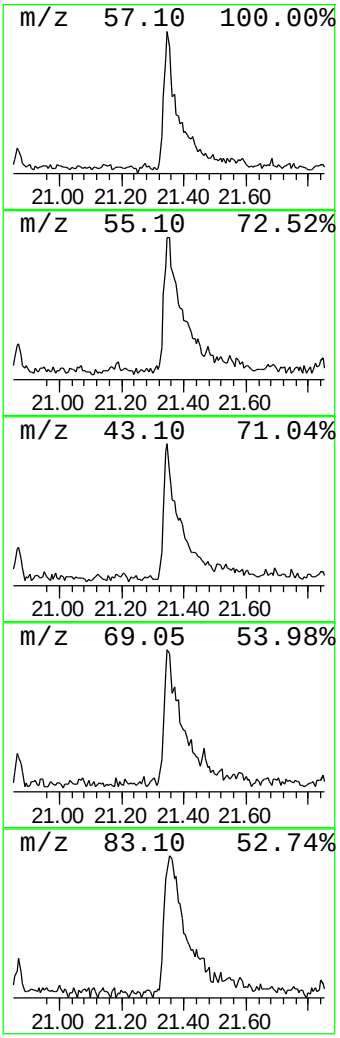
****

Peak Number 7 Hexacosyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.35	4.37 ng	280524	Chrysene-d12	21.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	91
2	Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	91
3	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
4	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
5	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	91





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...	5.17	3.3	ng	65235	1	8.06	400230	20.0
unknown7.59	7.59	82.8	ng	1657260	1	8.06	400230	20.0
n-Hexadecanoic acid	18.31	2.7	ng	146366	4	17.43	1099740	20.0
Hexadecanoic acid...	19.73	3.8	ng	243043	5	21.69	1284150	20.0
Butyl myristate	20.77	2.9	ng	189042	5	21.69	1284150	20.0
Hexacosyl trifluo...	21.35	4.4	ng	280524	5	21.69	1284150	20.0