LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022619\
Data File : BG039613.D
Acq On : 26 Feb 2019 23:18
Operator : JU/SJ
Sample : K1594-28
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-3(8-9)

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-BG012919.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	3.222	18	23	32	rBV	83642	166490	6.86%	1.051%
2	3.293	32	35	42	rVB	34753	52937	2.18%	0.334%
3	5.713	436	447	455	rBV	581542	946232	38.98%	5.973%
4	7.311	710	719	731	rBV	609380	1069009	44.04%	6.748%
5	7.693	776	784	792	rBV	566934	987798	40.69%	6.235%
6	8.169	858	865	876	rVB	186440	326549	13.45%	2.061%
7	8.492	913	920	927	rBV	410408	707029	29.13%	4.463%
8	8.791	964	971	978	rBV4	12941	25920	1.07%	0.164%
9	9.344	1058	1065	1073	rBV	339731	615407	25.35%	3.885%
10	10.659	1281	1289	1297	rVB2	17189	29311	1.21%	0.185%
11	10.988	1331	1345	1353	rBV	257464	488158	20.11%	3.081%
12	11.088	1358	1362	1370	rVB6	15572	30930	1.27%	0.195%
13	11.176	1370	1377	1383	rBV2	14048	25769	1.06%	0.163%
14	13.414	1749	1758	1764	rBV	909153	1423451	58.64%	8.985%
15	14.231	1892	1897	1904	rVB	50856	74080	3.05%	0.468%
16	14.789	1982	1992	2002	rBV2	422521	696154	28.68%	4.394%
17	16.275	2238	2245	2255	rBV	800325	1277562	52.63%	8.064%
18	17.532	2453	2459	2470	rBV2	644877	983884	40.53%	6.210%
19	18.384	2597	2604	2613	rBV2	86496	148073	6.10%	0.935%
20	19.647	2813	2819	2825	rBV6	16375	33281	1.37%	0.210%
21	20.123	2894	2900	2906	rBV	1847748	2427386	100.00%	15.322%
22	20.393	2941	2946	2950	rBV5	18013	25146	1.04%	0.159%
23	21.415	3115	3120	3135	rBV3	100628	230822	9.51%	1.457%
24	21.668	3158	3163	3170	rVB	120731	163101	6.72%	1.030%
25	21.821	3181	3189	3200	rVB2	676865	1159335	47.76%	7.318%
26	21.968	3211	3214	3219	rVB	31630	43379	1.79%	0.274%
27	22.596	3316	3321	3326	rVB2	37449	62195	2.56%	0.393%
28	23.319	3437	3444	3452	rBV2	61042	119563	4.93%	0.755%
29	23.518	3472	3478	3485	rVB2	64926	125916	5.19%	0.795%
30	24.159	3579	3587	3593	rBV2	45368	103358	4.26%	0.652%
31	25.199	3749	3764	3779	rVB2	371112	1196233	49.28%	7.551%
32	26.332	3950	3957	3969	rVB5	25726	77990	3.21%	0.492%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022619\
Data File : BG039613.D
Acq On : 26 Feb 2019 23:18
Operator : JU/SJ
Sample : K1594-28
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-3(8-9)

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-BG012919.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

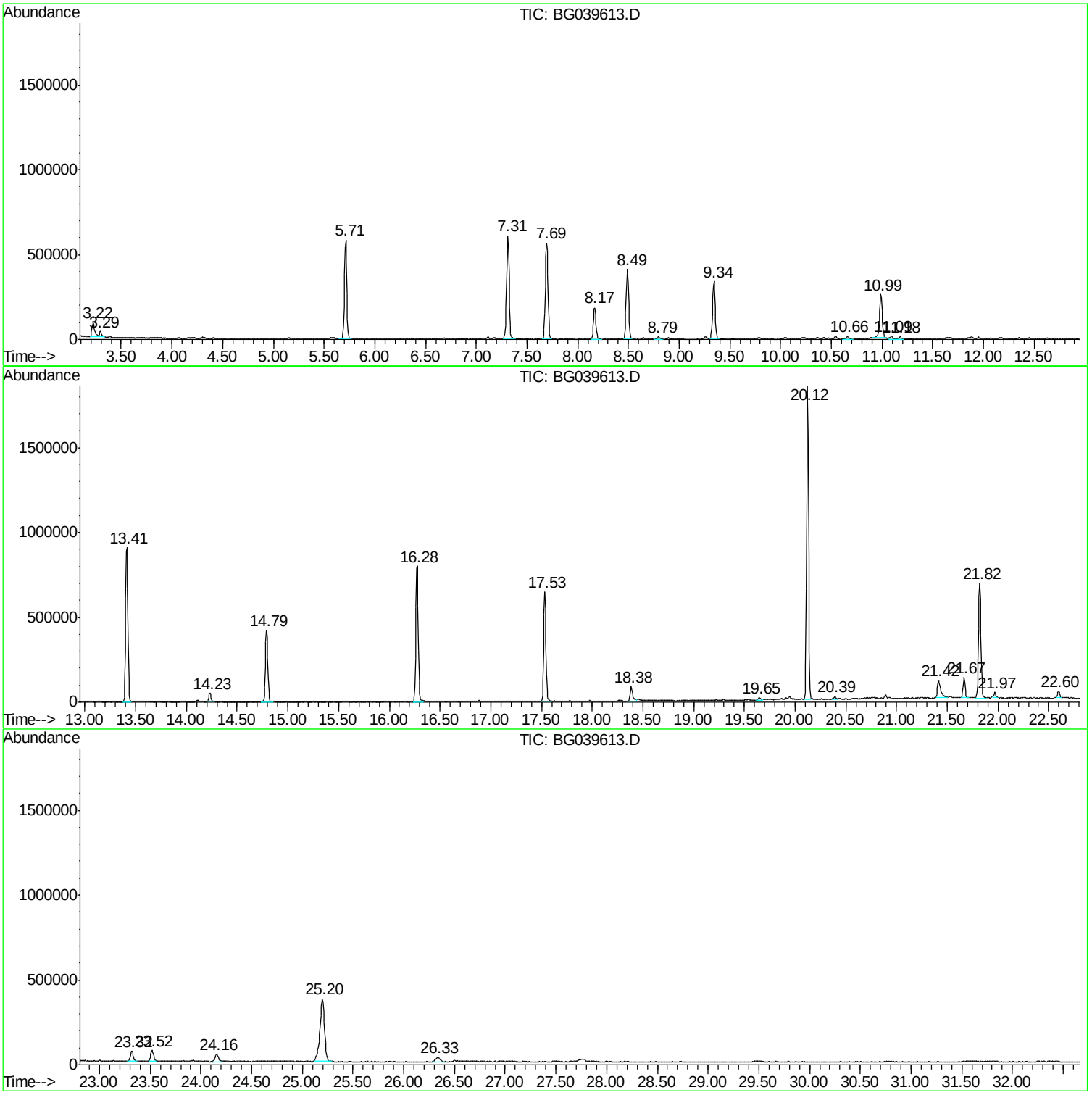
Sum of corrected areas: 15842448

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022619\
Data File : BG039613.D
Acq On : 26 Feb 2019 23:18
Operator : JU/SJ
Sample : K1594-28
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-3(8-9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.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

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022619\
Data File : BG039613.D
Acq On : 26 Feb 2019 23:18
Operator : JU/SJ
Sample : K1594-28
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-3(8-9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

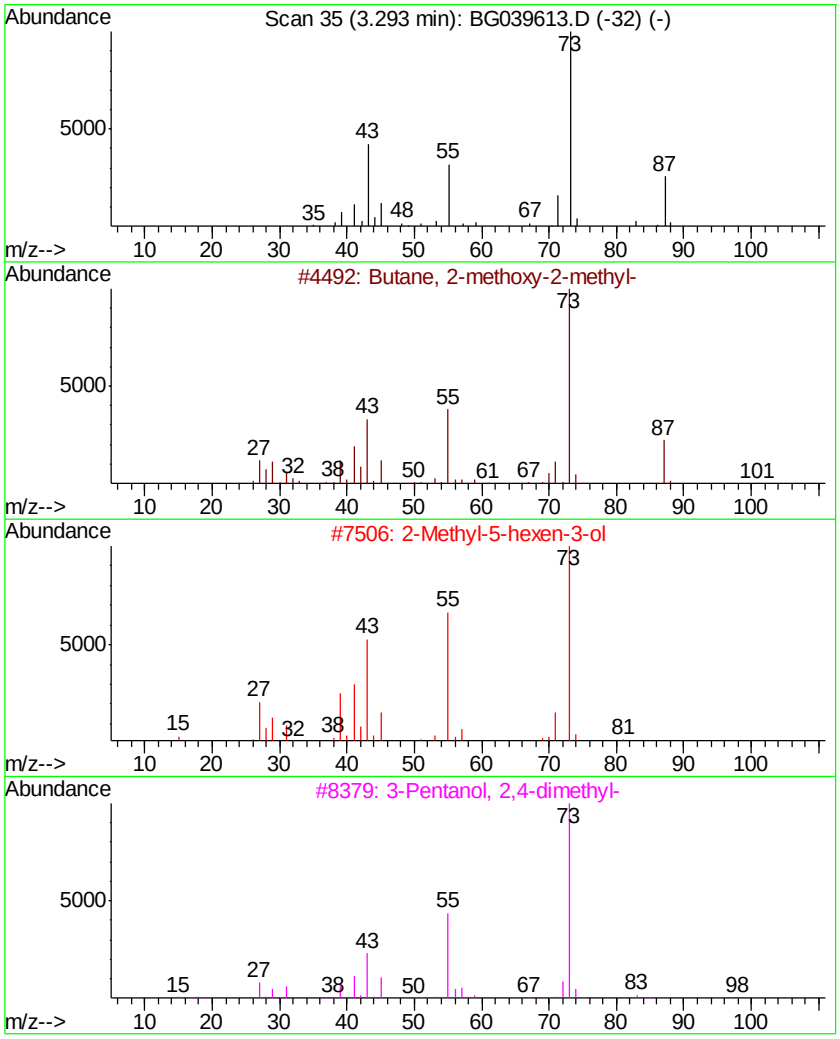
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

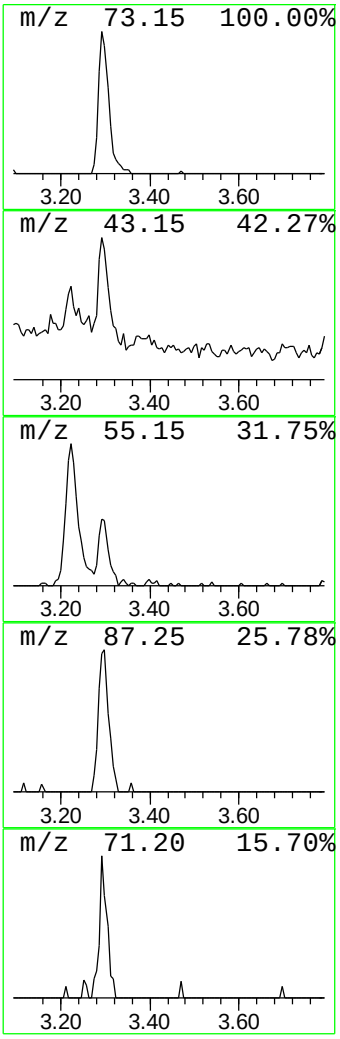
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.29	3.24 ng	52937	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022619\
Data File : BG039613.D
Acq On : 26 Feb 2019 23:18
Operator : JU/SJ
Sample : K1594-28
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-3(8-9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

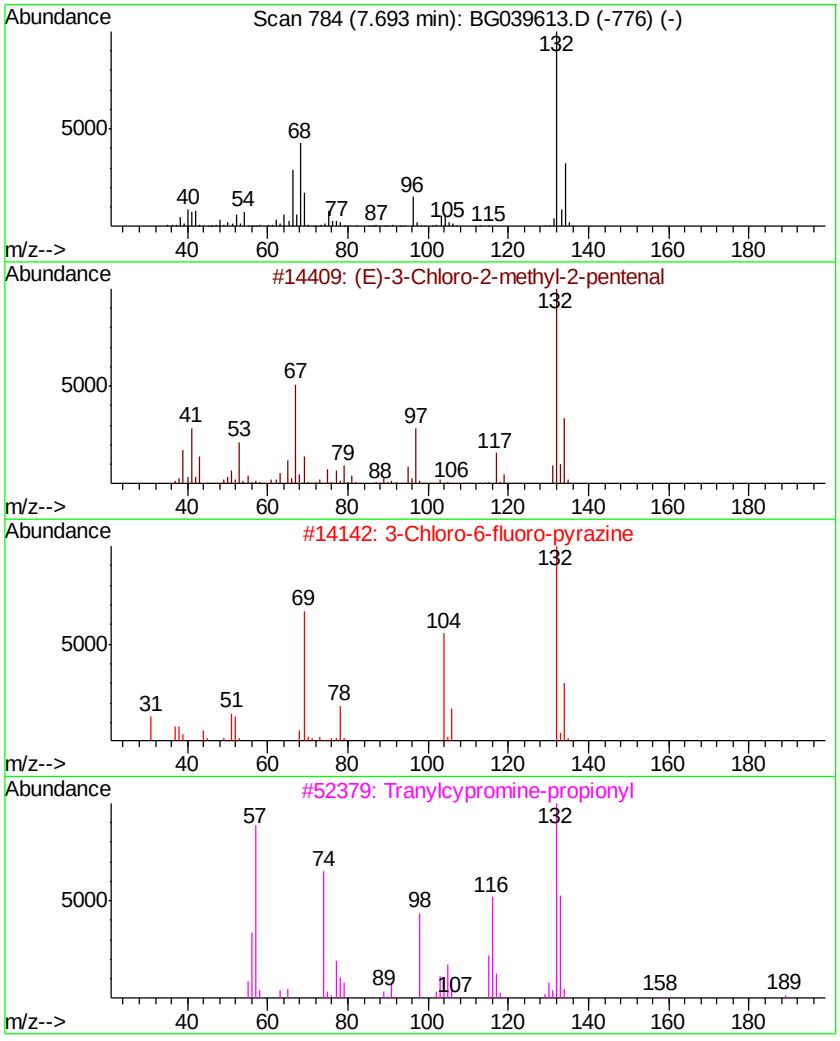
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

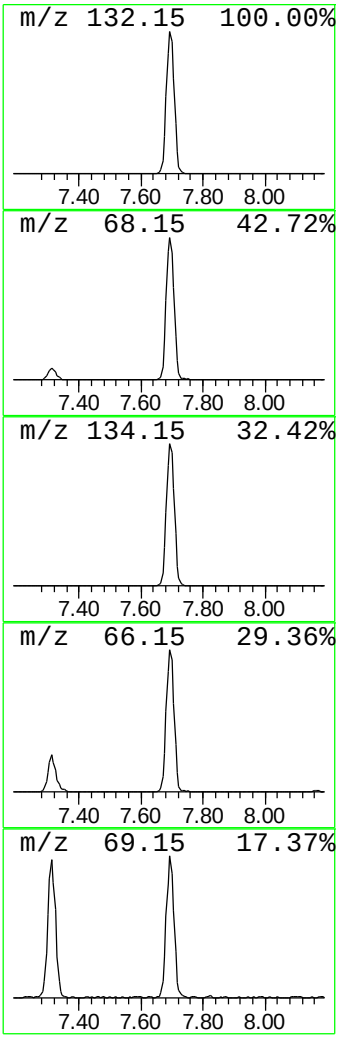
****

Peak Number 3 unknown7.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.69	60.50 ng	987798	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022619\
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Sample : K1594-28
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-3(8-9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

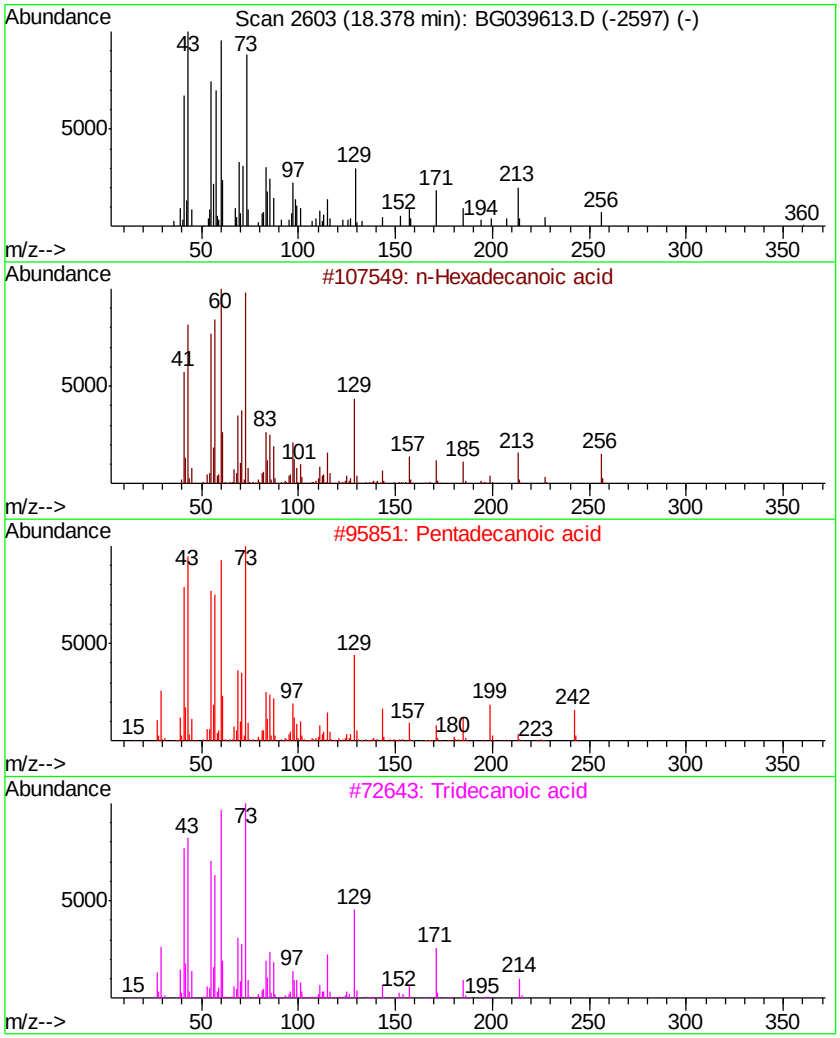
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

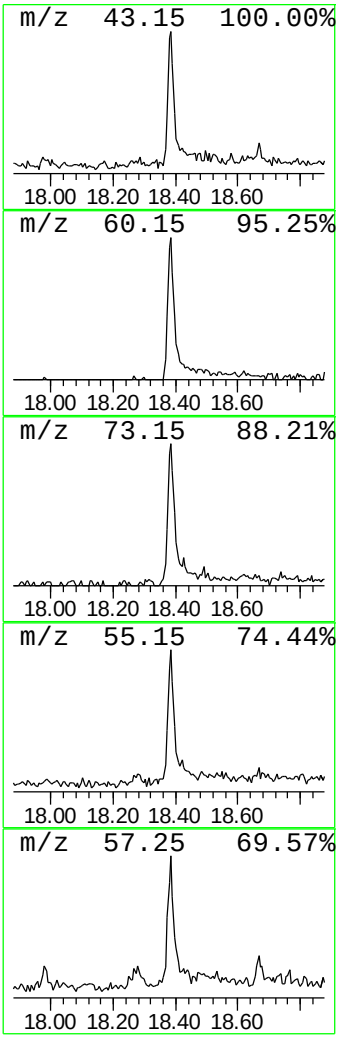
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.38	3.01 ng	148073	Phenanthrene-d10	17.53

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	72
5	Octadecanoic acid	284	C18H36O2	000057-11-4	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022619\
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Sample : K1594-28
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Instrument : BNA_G
ClientSampleId : B-3(8-9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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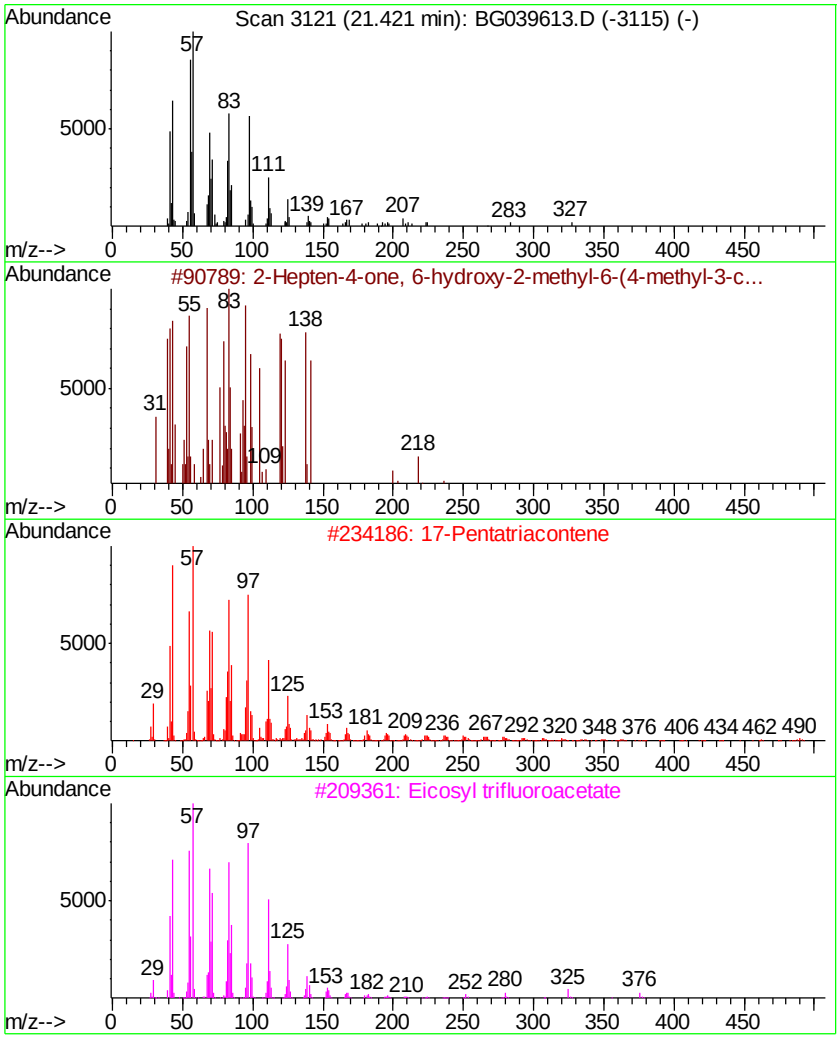
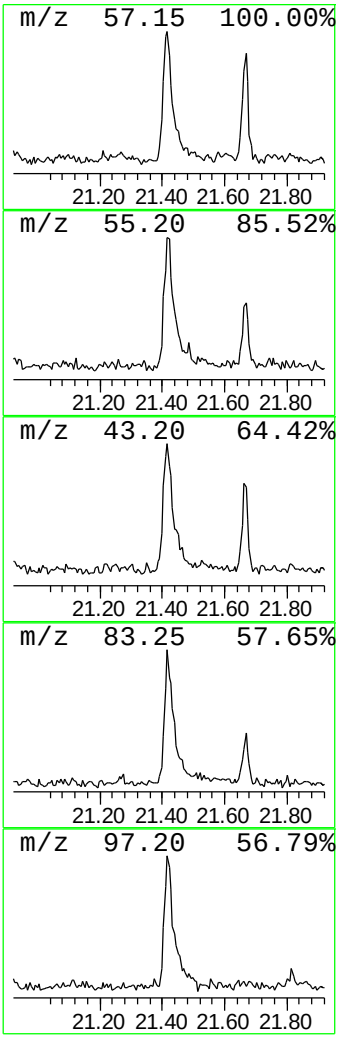
****

Peak Number 6 2-Hepten-4-one, 6-hydroxy-2... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.42	3.98 ng	230822	Chrysene-d12	21.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hepten-4-one, 6-hydroxy-2-meth...	236	C15H24O2	038043-98-0	92
2	17-Pentatriacontene	491	C35H70	006971-40-0	86
3	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	83
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	83
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	83





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Sample : K1594-28
Misc :
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Instrument : BNA_G
ClientSampleId : B-3(8-9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

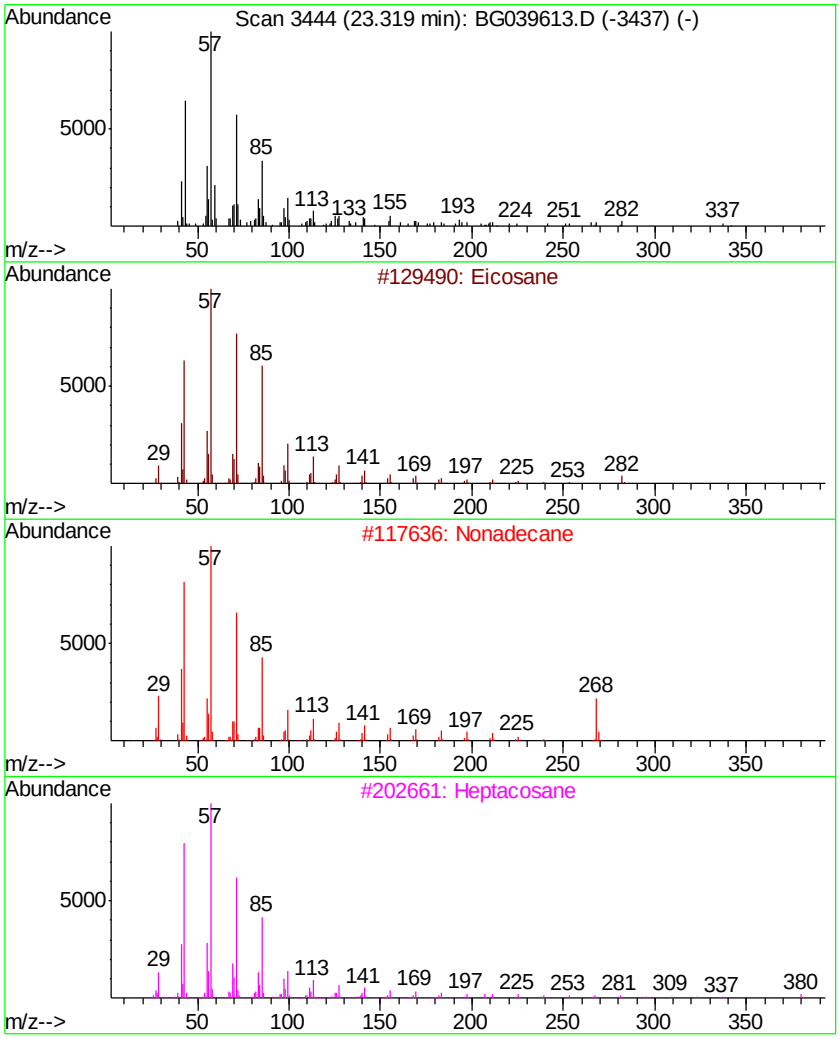
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

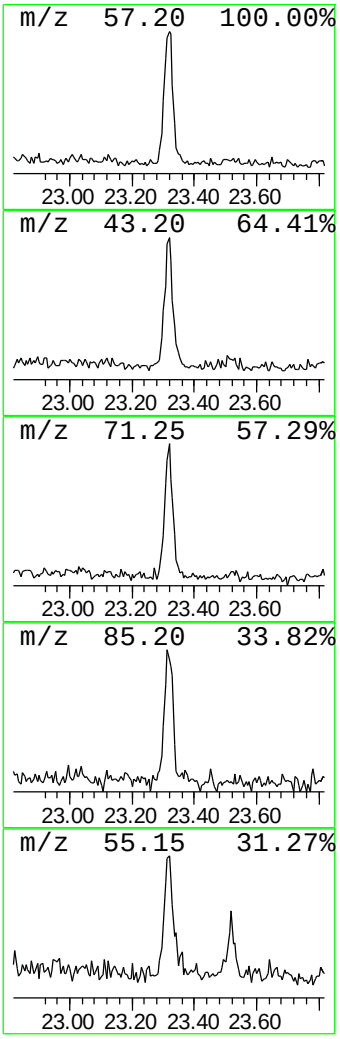
****

Peak Number 7 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.32	2.06 ng	119563	Chrysene-d12	21.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	Nonadecane	268	C19H40	000629-92-5	92
3	Heptacosane	380	C27H56	000593-49-7	76
4	Heneicosane	296	C21H44	000629-94-7	76
5	Octacosane	394	C28H58	000630-02-4	76





Library Search Compound Report

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Misc :
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Instrument : BNA_G
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

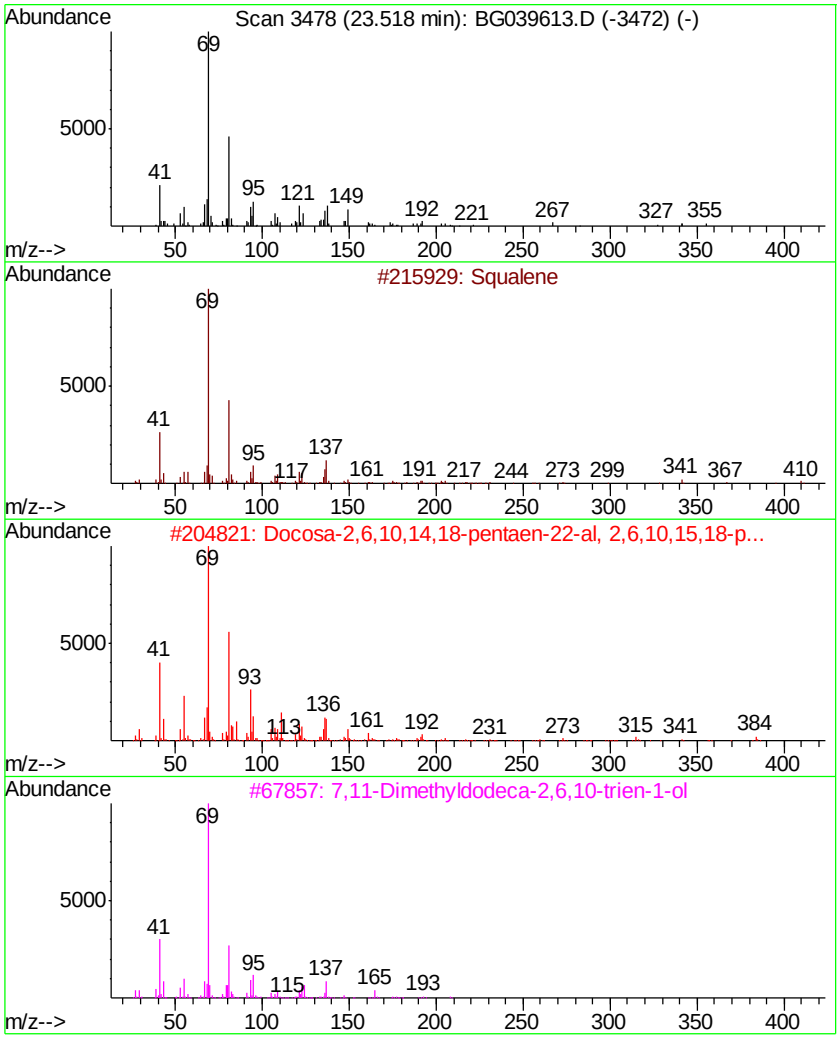
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

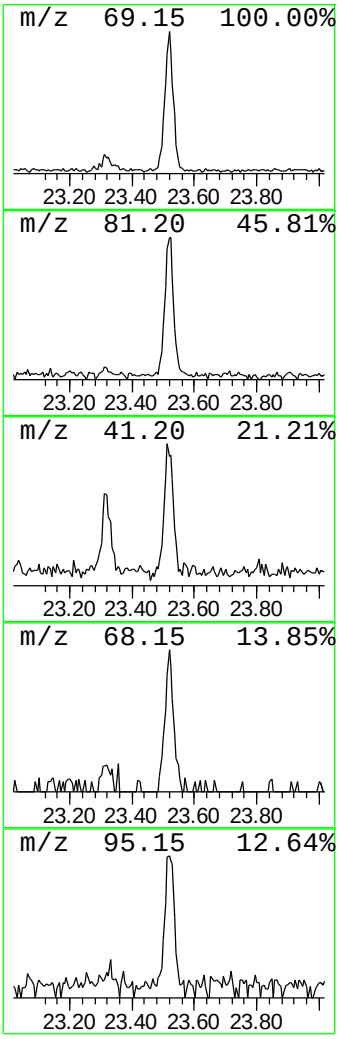
****

Peak Number 8 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.52	2.11 ng	125916	Perylene-d12	25.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	80
4	Supraene	410	C30H50	007683-64-9	80
5	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_G
ClientSampleId : B-3(8-9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
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
Butane, 2-methoxy...	3.29	3.2	ng	52937	1	8.17	326549	20.0
unknown7.69	7.69	60.5	ng	987798	1	8.17	326549	20.0
n-Hexadecanoic acid	18.38	3.0	ng	148073	4	17.53	983884	20.0
2-Hepten-4-one, 6...	21.42	4.0	ng	230822	5	21.82	1159340	20.0
Eicosane	23.32	2.1	ng	119563	5	21.82	1159340	20.0
Squalene	23.52	2.1	ng	125916	6	25.19	1196230	20.0