LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG032219\
Data File : BG040085.D
Acq On : 22 Mar 2019 16:14
Operator : JU/SJ
Sample : K2040-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S4B(22-28)

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-BG030419.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	3.195	12	18	26	rBV	97191	210340	7.07%	1.153%
2	3.272	26	31	41	rVV	180515	267129	8.98%	1.465%
3	3.372	41	48	58	rVB	164842	329799	11.09%	1.808%
4	5.692	434	443	456	rBV	891680	1422473	47.82%	7.799%
5	7.296	706	716	728	rBV	895110	1573627	52.91%	8.628%
6	7.672	772	780	793	rVB	869238	1488765	50.05%	8.163%
7	8.142	853	860	869	rBV	157904	269090	9.05%	1.475%
8	8.465	908	915	923	rVB	615944	1079989	36.31%	5.921%
9	9.322	1053	1061	1072	rBV	524884	936039	31.47%	5.132%
10	10.961	1333	1340	1350	rBV	202248	366120	12.31%	2.007%
11	13.393	1746	1754	1762	rVB	1322609	2042960	68.69%	11.201%
12	14.210	1887	1893	1901	rBV	102503	149562	5.03%	0.820%
13	14.768	1981	1988	1997	rBV2	326604	523879	17.61%	2.872%
14	16.254	2235	2241	2253	rBV	1121452	1731674	58.22%	9.494%
15	17.517	2449	2456	2461	rBV	437217	671266	22.57%	3.680%
16	18.369	2595	2601	2607	rBV2	46349	77205	2.60%	0.423%
17	20.108	2891	2897	2903	rBV	2226931	2974342	100.00%	16.308%
18	21.394	3111	3116	3145	rBV3	76758	299116	10.06%	1.640%
19	21.805	3178	3186	3197	rBV	490237	800630	26.92%	4.390%
20	23.280	3430	3437	3444	rBV4	24458	48518	1.63%	0.266%
21	24.108	3573	3578	3588	rVB3	31220	63893	2.15%	0.350%
22	25.107	3737	3748	3749	rBV5	26464	64920	2.18%	0.356%
23	25.172	3749	3759	3771	rVB2	254706	787797	26.49%	4.319%
24	26.276	3938	3947	3956	rVB8	19985	59847	2.01%	0.328%

Sum of corrected areas: 18238980

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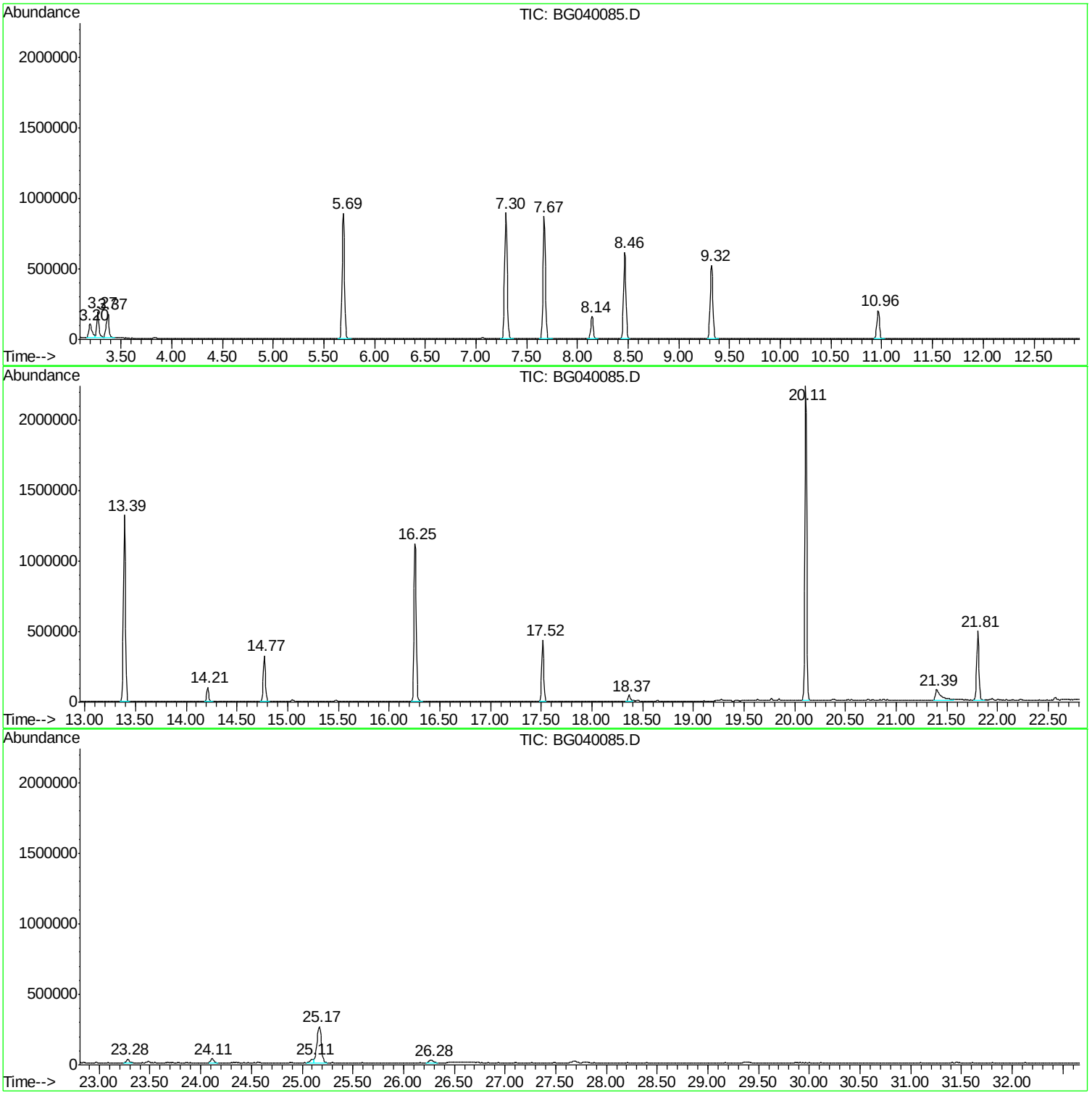
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S4B(22-28)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.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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ClientSampleId : S4B(22-28)

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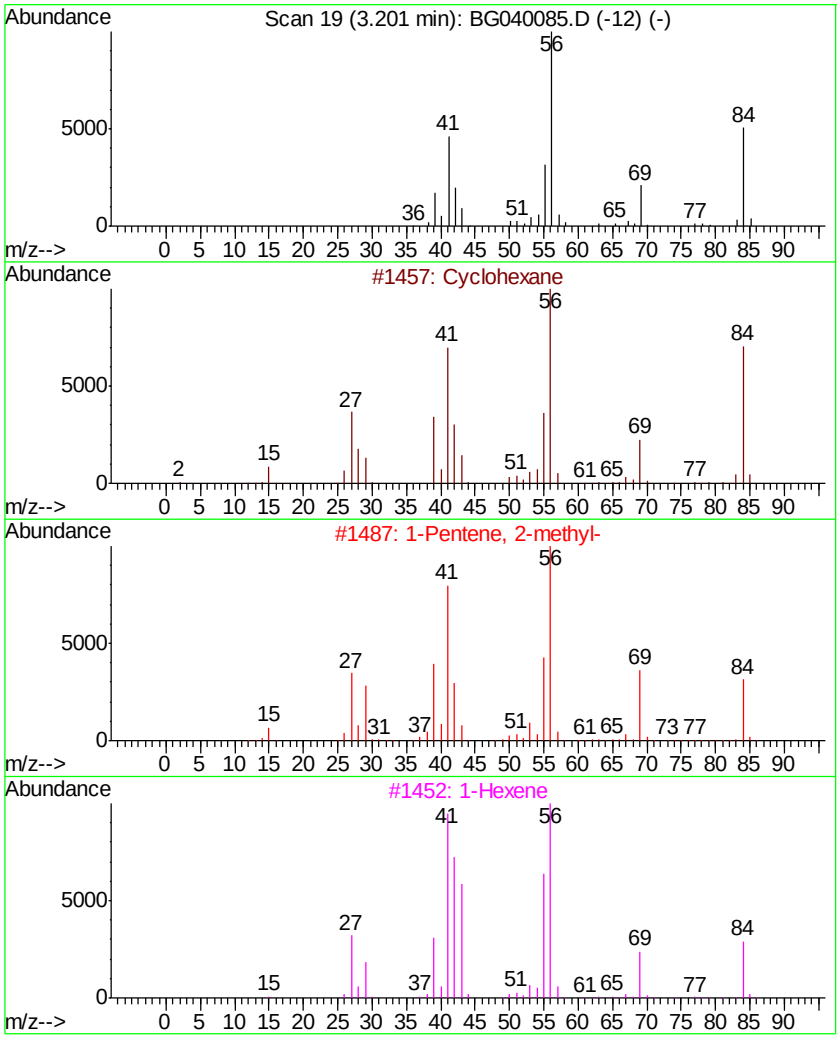
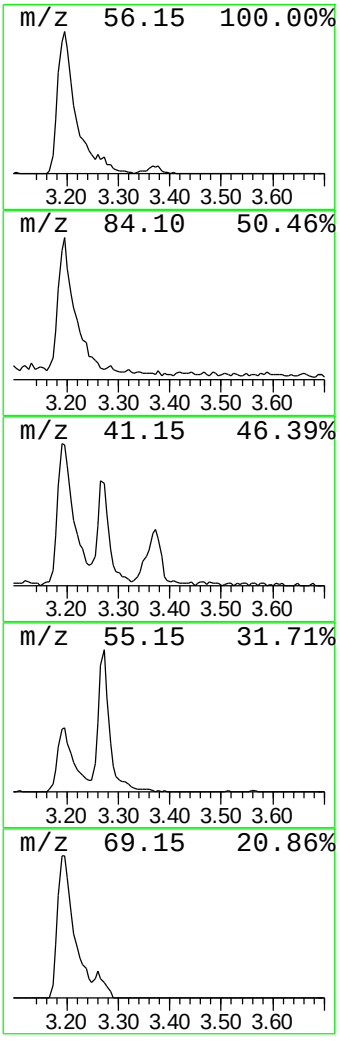
****

Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.20	15.63 ng	210340	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	91
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	78
3	1-Hexene	84	C6H12	000592-41-6	53
4	1-Butanol	74	C4H10O	000071-36-3	50
5	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	47





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Operator : JU/SJ
Sample : K2040-05
Misc :
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Instrument : BNA_G
ClientSampleId : S4B(22-28)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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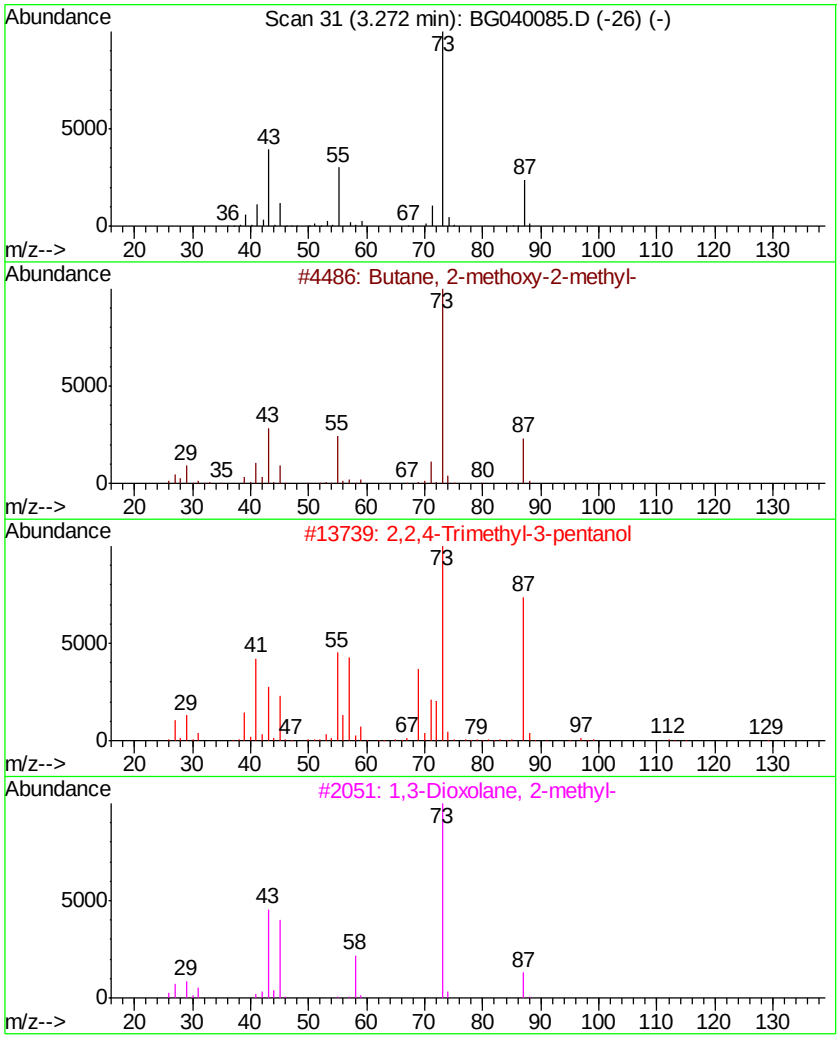
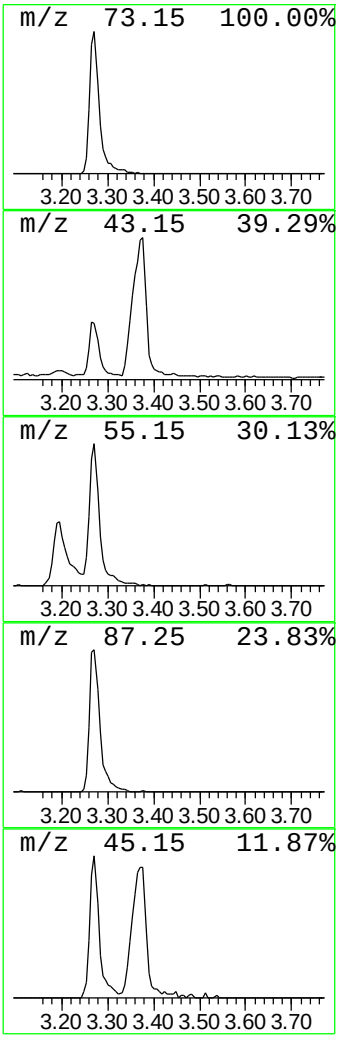
Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.27	19.85 ng	267129	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG032219\
Data File : BG040085.D
Acq On : 22 Mar 2019 16:14
Operator : JU/SJ
Sample : K2040-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S4B(22-28)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

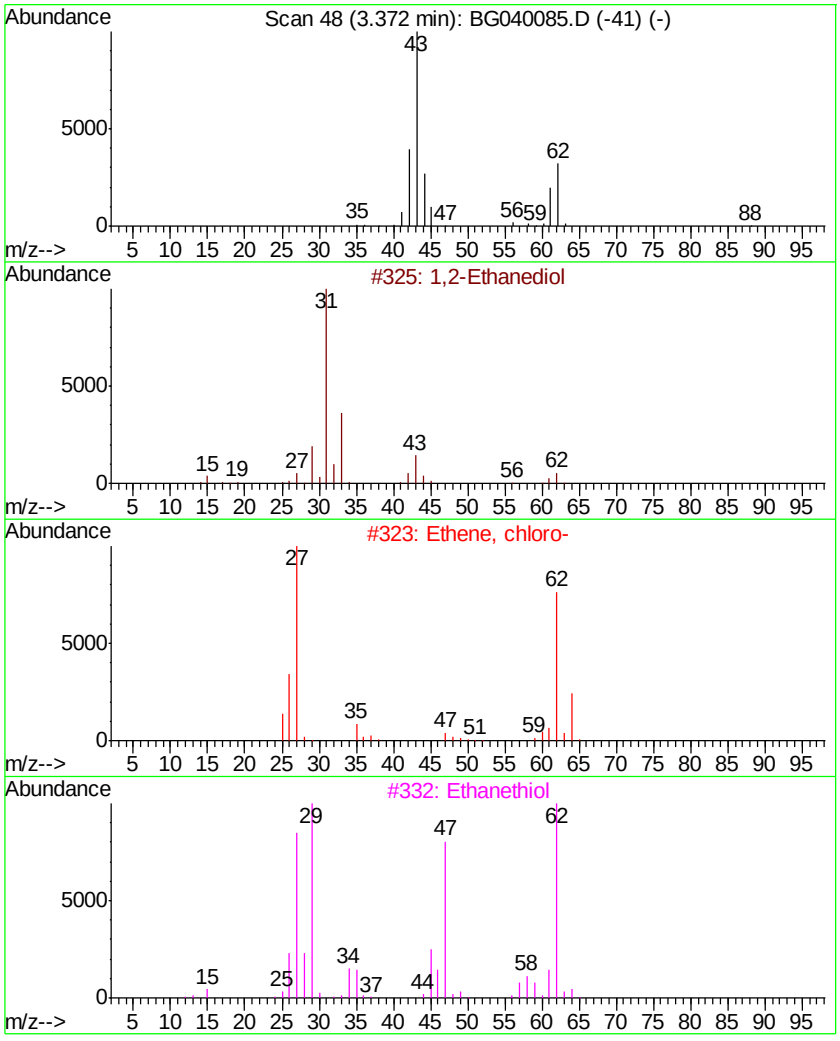
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

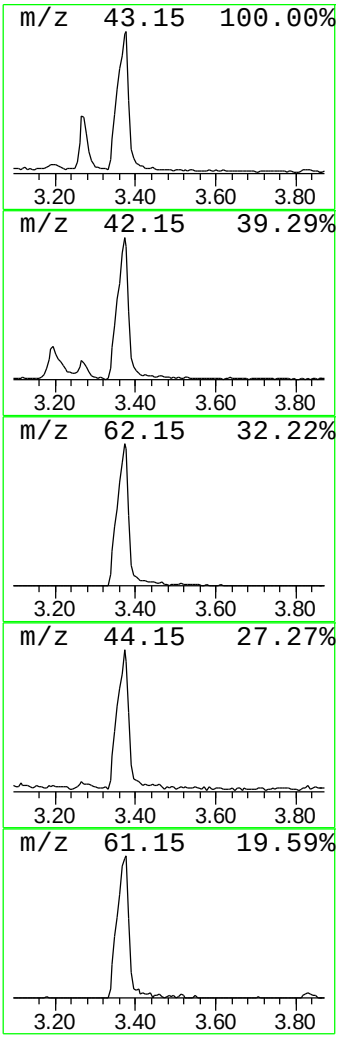
****

Peak Number 3 unknown3.37 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.37	24.51 ng	329799	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Ethanediol	62	C2H6O2	000107-21-1	9
2	Ethene, chloro-	62	C2H3Cl	000075-01-4	7
3	Ethanethiol	62	C2H6S	000075-08-1	5
4	Formic acid, propyl ester	88	C4H8O2	000110-74-7	4
5	Peroxide, dimethyl	62	C2H6O2	000690-02-8	4





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Data File : BG040085.D
Acq On : 22 Mar 2019 16:14
Operator : JU/SJ
Sample : K2040-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S4B(22-28)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

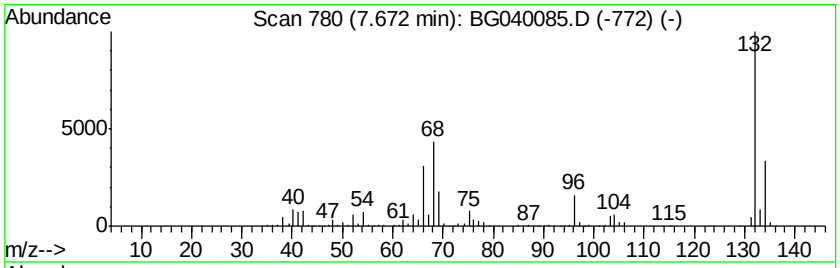
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

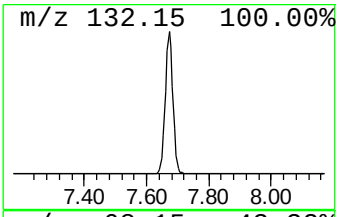
****

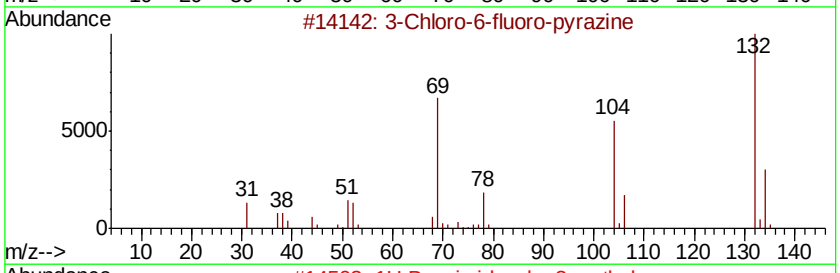
Peak Number 4 unknown7.67 Concentration Rank 1

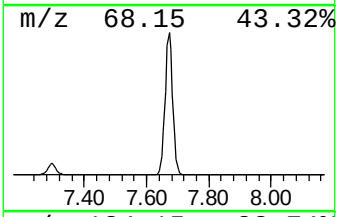
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.67	110.65 ng	1488770	1,4-Dichlorobenzene-d4	8.14

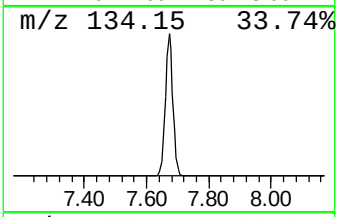
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12

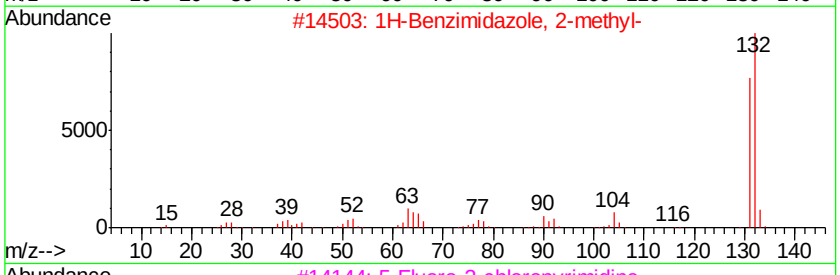


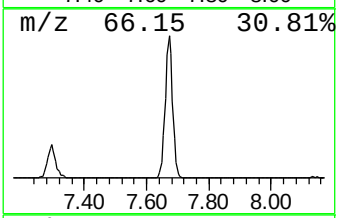


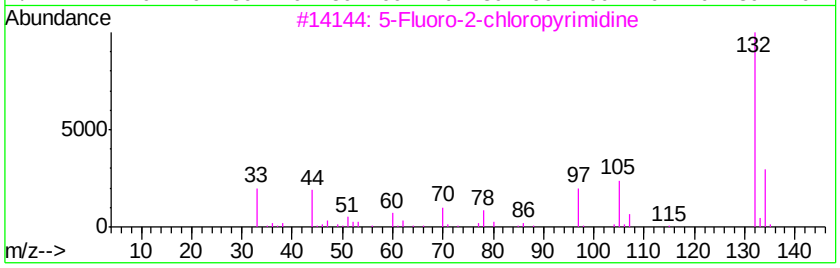


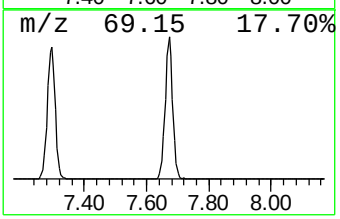












Library Search Compound Report

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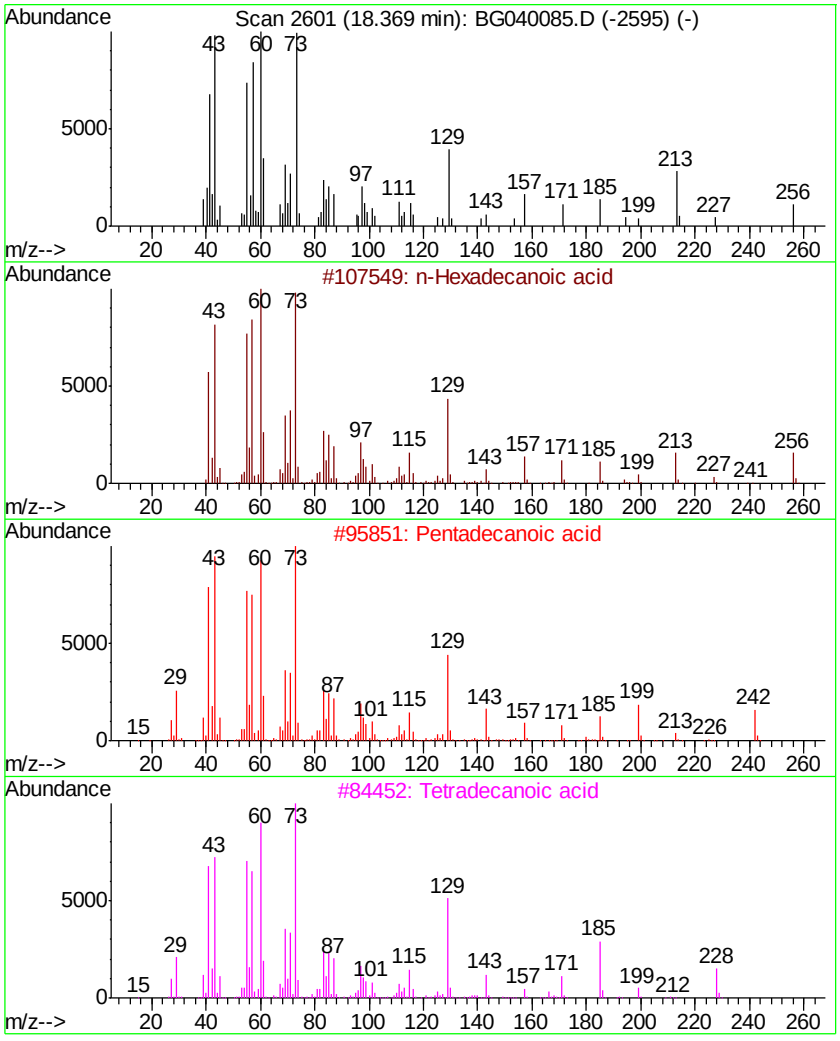
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

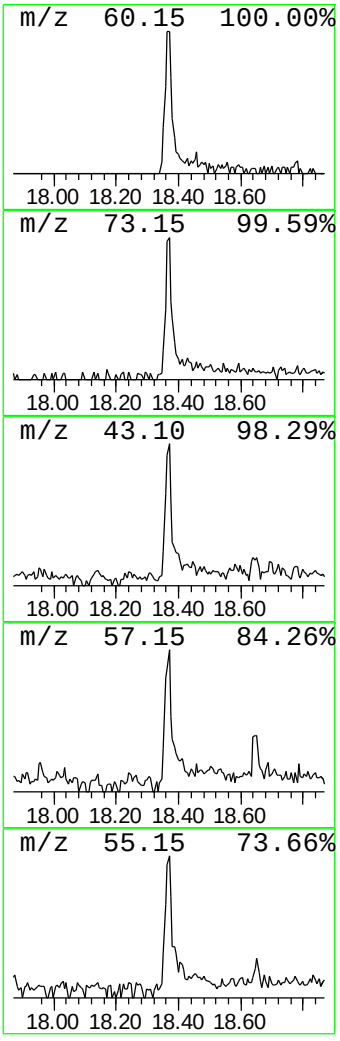
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.37	2.30 ng	77205	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	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	Lactose	342	C12H22O11	000063-42-3	52





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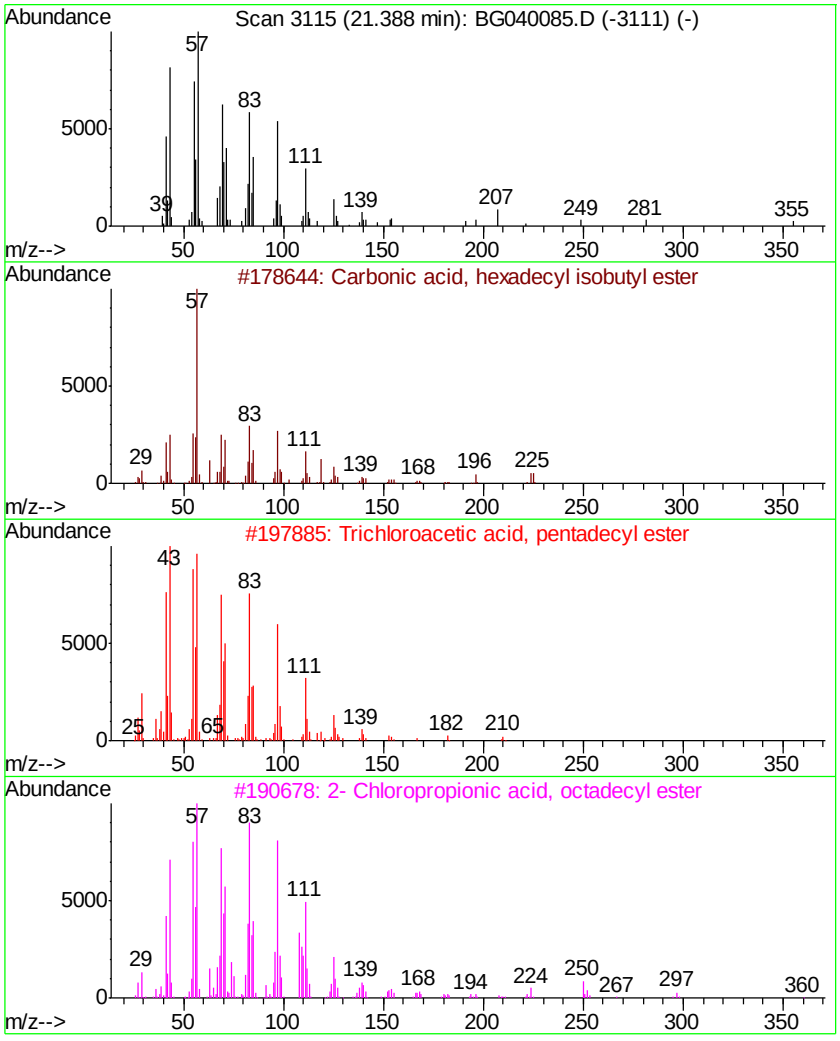
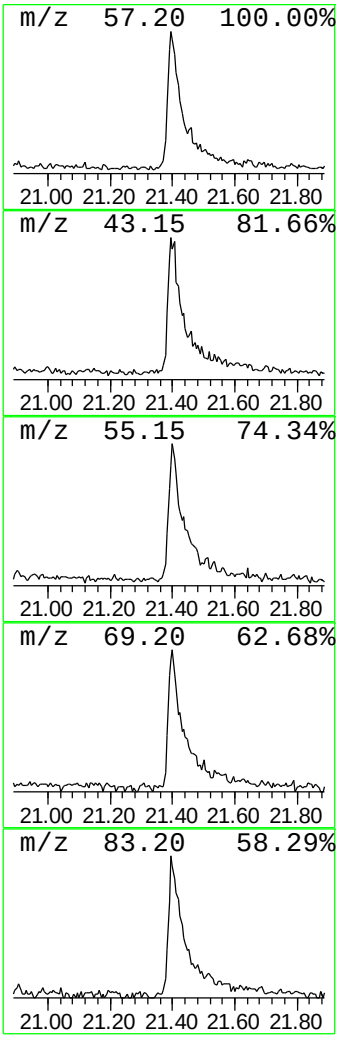
****

Peak Number 7 Carbonic acid, hexadecyl is... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.39	7.47 ng	299116	Chrysene-d12	21.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, hexadecyl isobutyl...	342	C21H42O3	1000314-61-3	91
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	90
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1-Pentene, 2-methyl-	3.20	15.6	ng	210340	1	8.14	269090	20.0
Butane, 2-methoxy...	3.27	19.9	ng	267129	1	8.14	269090	20.0
unknown3.37	3.37	24.5	ng	329799	1	8.14	269090	20.0
unknown7.67	7.67	110.7	ng	1488770	1	8.14	269090	20.0
n-Hexadecanoic acid	18.37	2.3	ng	77205	4	17.52	671266	20.0
Carbonic acid, he...	21.39	7.5	ng	299116	5	21.81	800630	20.0