LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110819\
Data File : BG043582.D
Acq On : 8 Nov 2019 23:11
Operator : JU
Sample : K5742-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-30-(6-8)

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-BG102119.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	3.172	9	14	23	rVB	96909	170250	7.85%	1.356%
2	4.183	180	186	200	rVB	289356	491123	22.64%	3.912%
3	5.105	338	343	356	rVB	100485	162267	7.48%	1.292%
4	5.599	419	427	444	rBV	463394	836531	38.56%	6.663%
5	7.203	691	700	723	rBV	499368	995024	45.86%	7.925%
6	7.549	752	759	771	rBV	530625	955529	44.04%	7.611%
7	8.002	829	836	846	rBV2	100069	174734	8.05%	1.392%
8	8.325	883	891	900	rBV	391118	716709	33.03%	5.708%
9	9.165	1026	1034	1051	rBV	278886	568930	26.22%	4.531%
10	10.810	1308	1314	1322	rBV	103978	209830	9.67%	1.671%
11	13.254	1722	1730	1742	rBV	806543	1340758	61.80%	10.679%
12	14.083	1865	1871	1885	rBV2	60232	115731	5.33%	0.922%
13	14.635	1958	1965	1978	rBV2	214913	351755	16.21%	2.802%
14	16.127	2212	2219	2234	rBV	765794	1292793	59.59%	10.297%
15	17.379	2426	2432	2442	rBV	244641	436277	20.11%	3.475%
16	19.988	2870	2876	2890	rBV	1534735	2169564	100.00%	17.280%
17	20.675	2984	2993	2996	rBV7	11916	22649	1.04%	0.180%
18	21.286	3093	3097	3112	rBV5	42650	127830	5.89%	1.018%
19	21.644	3149	3158	3168	rBV2	278551	531905	24.52%	4.236%
20	21.827	3184	3189	3193	rVB4	16945	26779	1.23%	0.213%
21	22.426	3287	3291	3297	rVB3	19933	29188	1.35%	0.232%
22	23.107	3400	3407	3415	rBV6	22709	50036	2.31%	0.399%
23	23.301	3434	3440	3447	rVB2	89148	174476	8.04%	1.390%
24	23.901	3537	3542	3549	rVB4	17345	32829	1.51%	0.261%
25	24.835	3689	3701	3715	rBV3	184135	571904	26.36%	4.555%

Sum of corrected areas: 12555401

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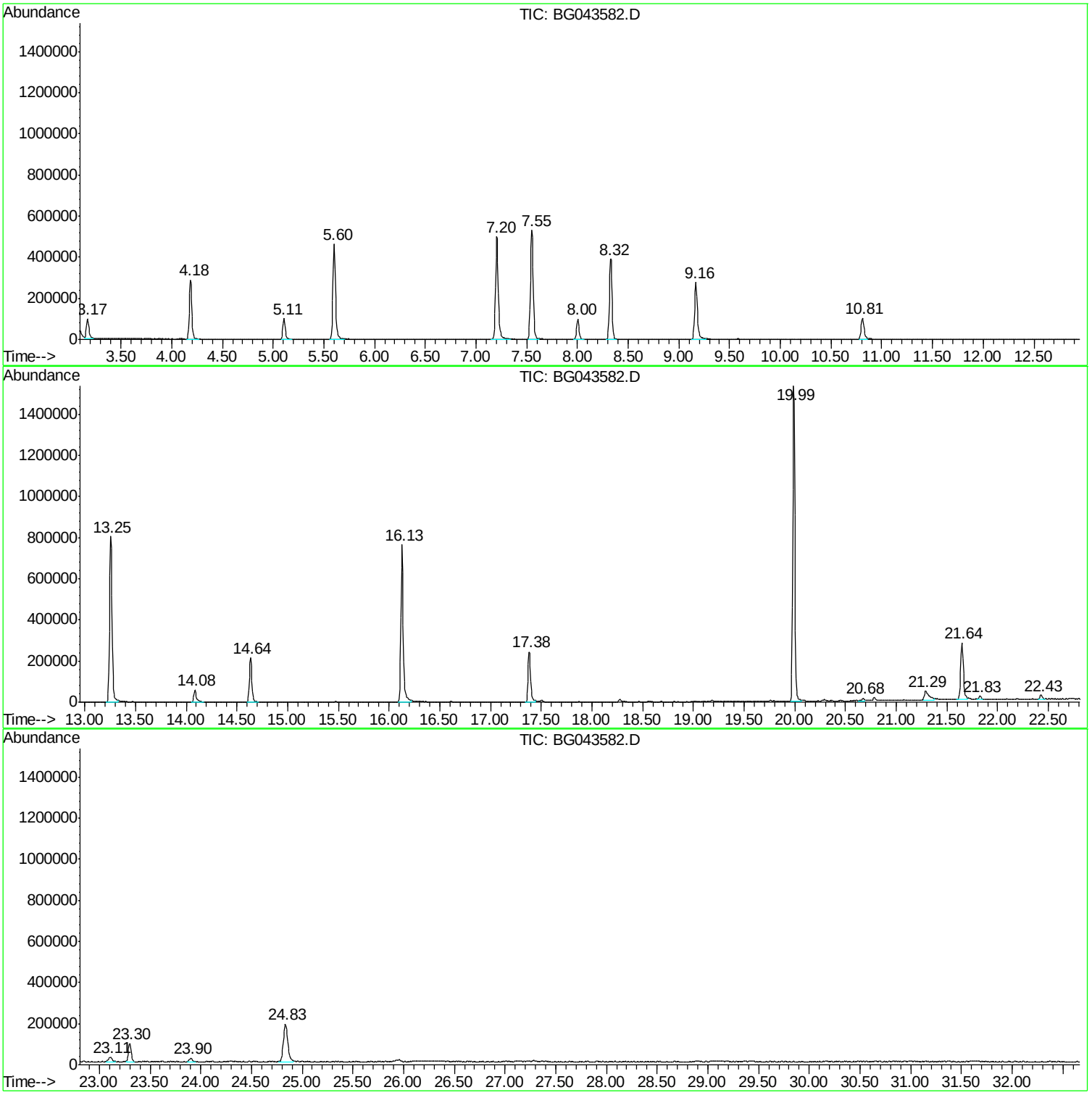
Instrument :
BNA_G
ClientSampleId :
SB-30-(6-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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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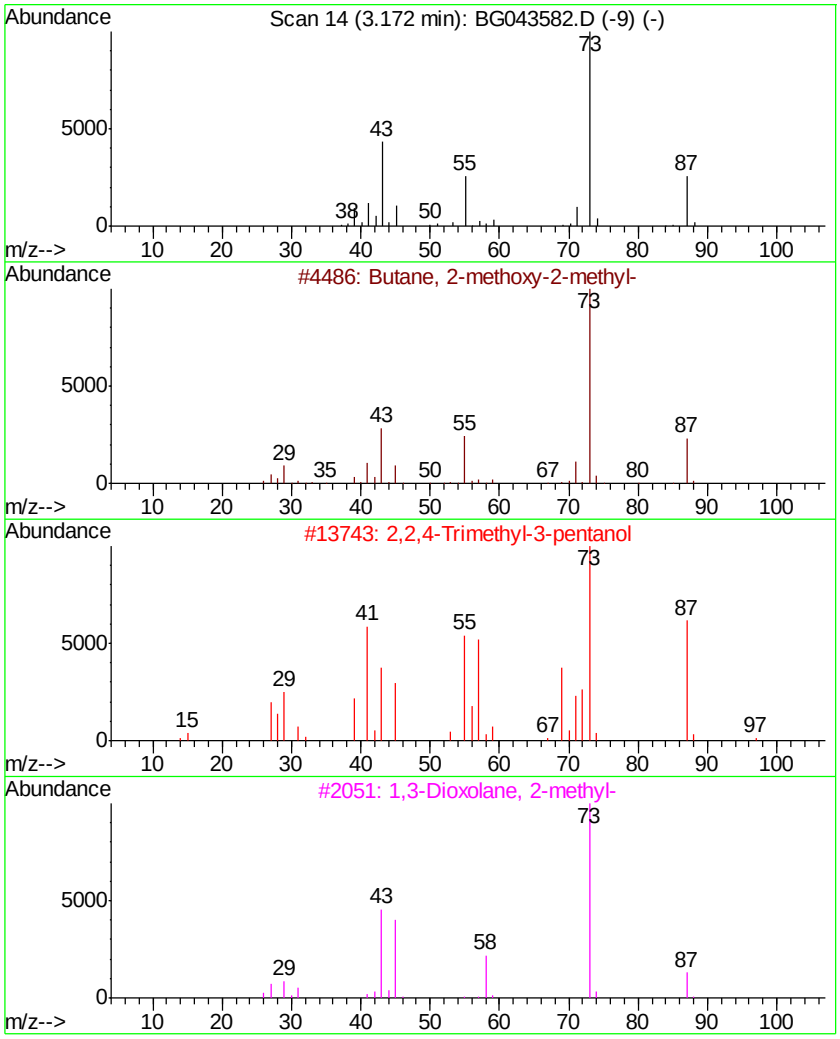
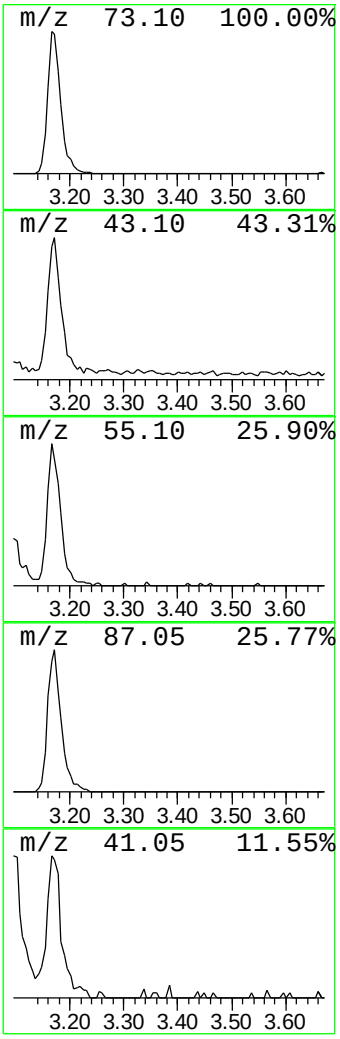
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	19.49 ng	170250	1,4-Dichlorobenzene-d4	8.00

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	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





Library Search Compound Report

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Data File : BG043582.D
Acq On : 8 Nov 2019 23:11
Operator : JU
Sample : K5742-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-30-(6-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

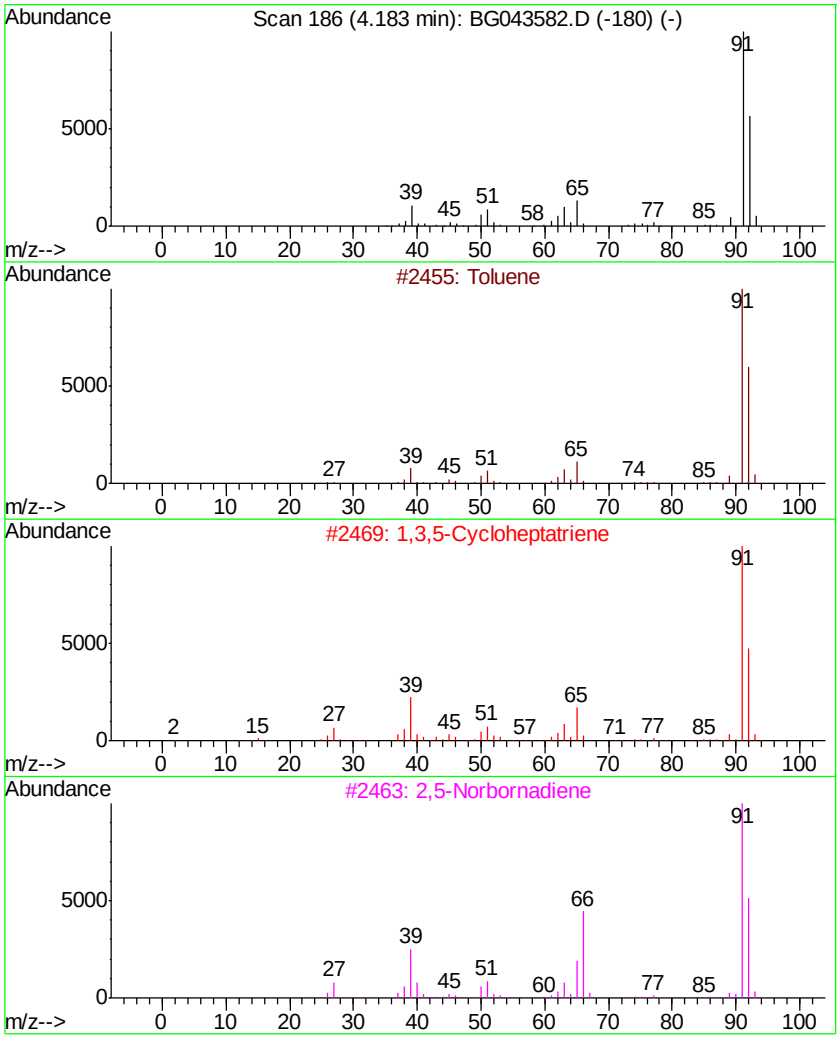
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

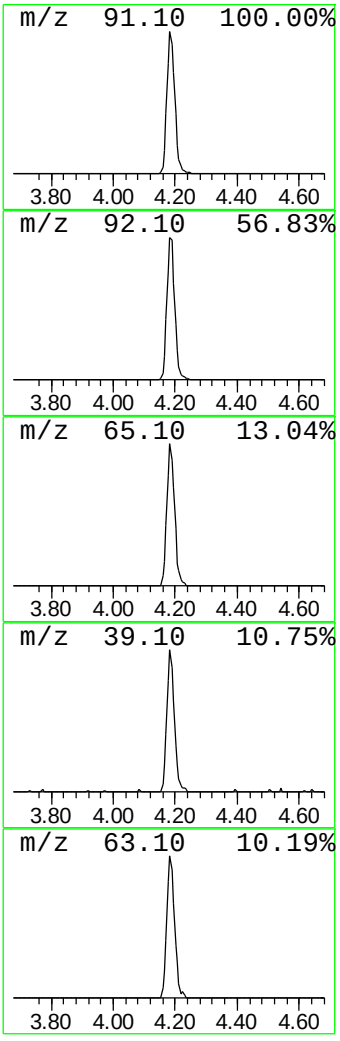
****

Peak Number 2 1,3,5-Cycloheptatriene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.18	56.21 ng	491123	1,4-Dichlorobenzene-d4	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Toluene	92	C7H8	000108-88-3	95
2	1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	90
3	2,5-Norbornadiene	92	C7H8	000121-46-0	83
4	Molybdenum, di-.mu.-chlorobis[(1...	532	C20H26Cl2Mo2	035625-66-2	72
5	Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	64





Library Search Compound Report

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Operator : JU
Sample : K5742-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-30-(6-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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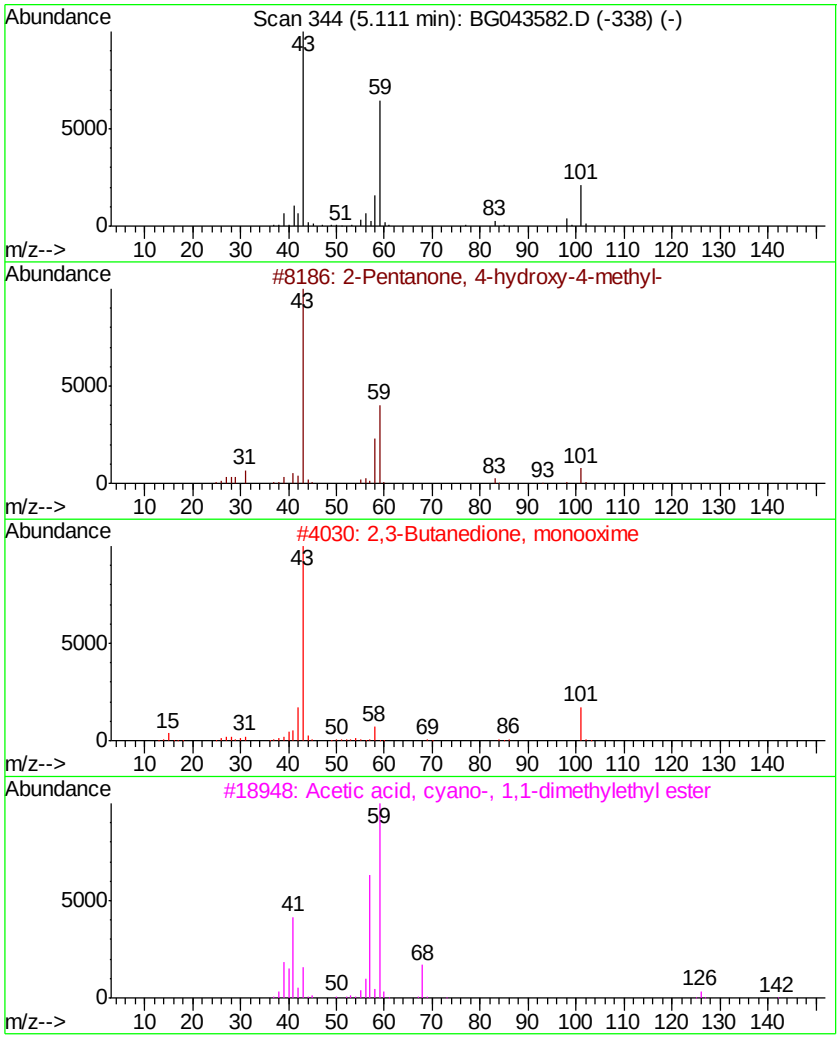
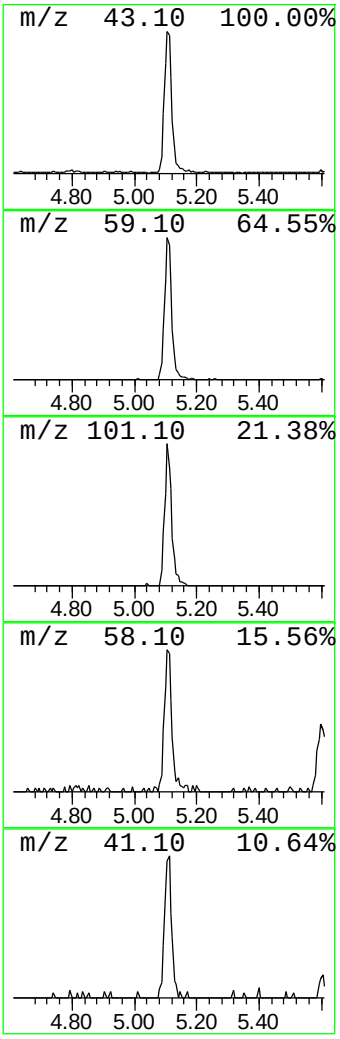
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	18.57 ng	162267	1,4-Dichlorobenzene-d4	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

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Sample : K5742-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-30-(6-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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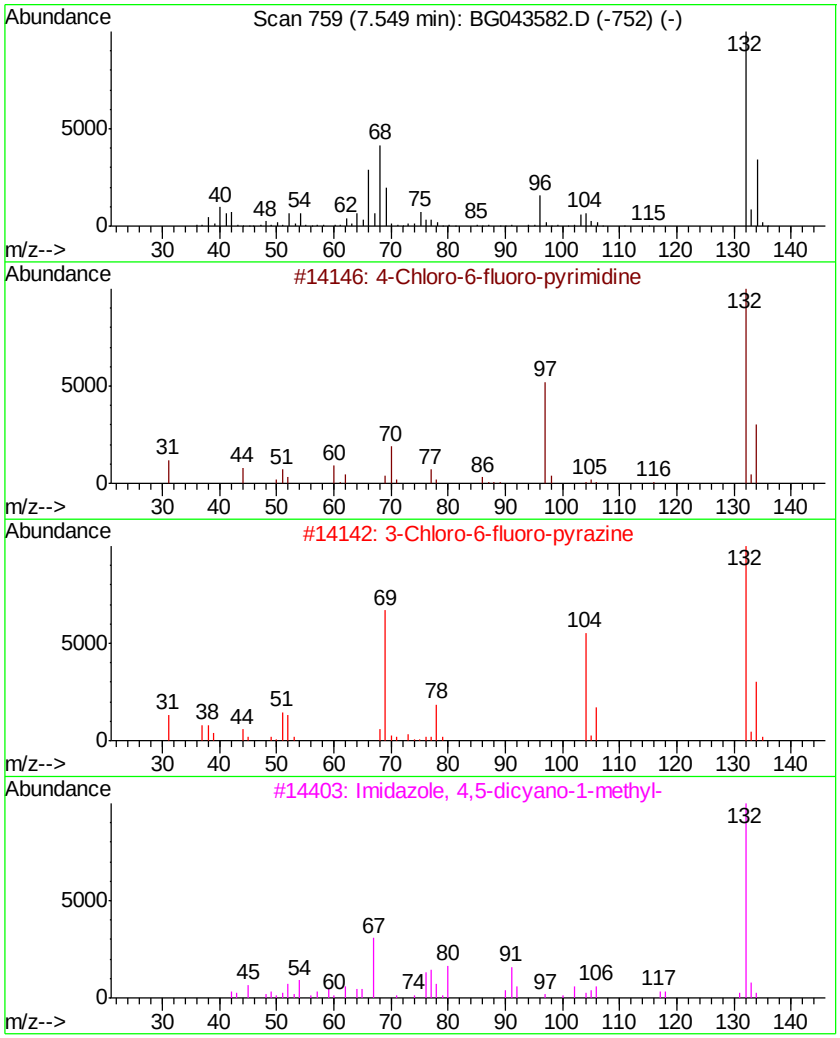
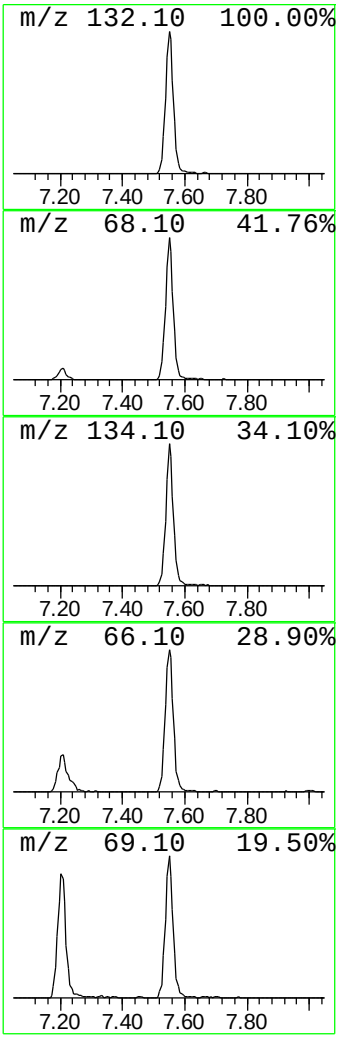
Peak Number 4 unknown7.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.55	109.37 ng	955529	1,4-Dichlorobenzene-d4	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	25
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-30-(6-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
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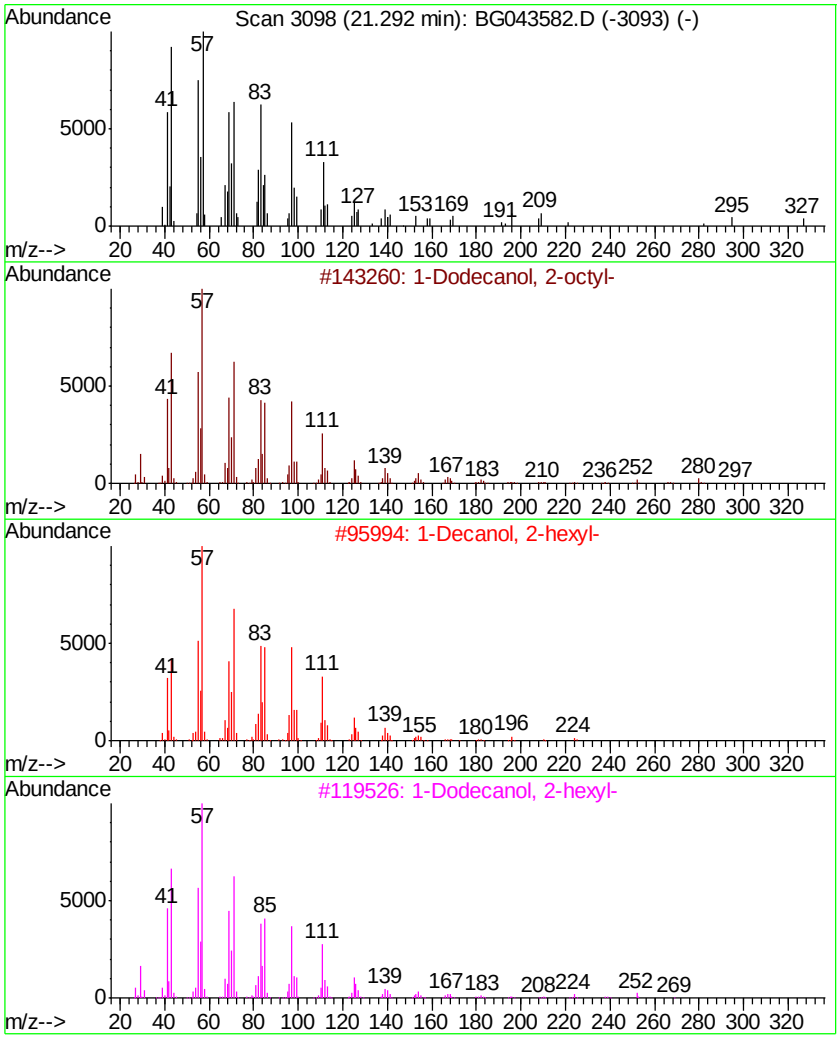
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

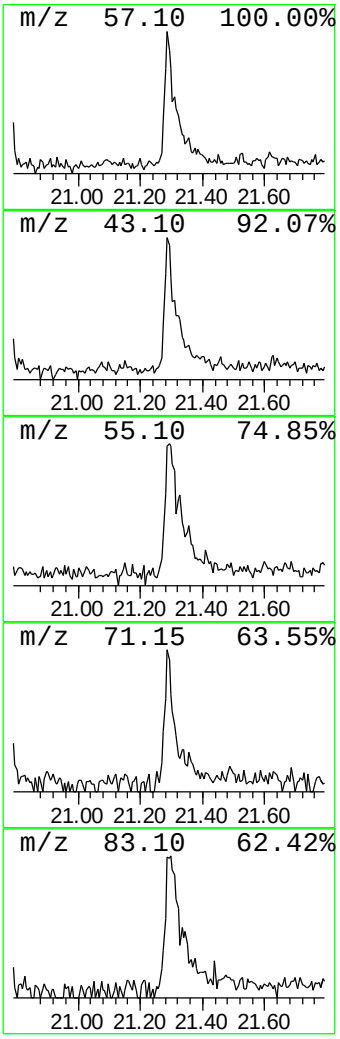
****

Peak Number 6 1-Dodecanol, 2-octyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.29	4.81 ng	127830	Chrysene-d12	21.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	87
2	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	87
3	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	80
4	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	80
5	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	72





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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-30-(6-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

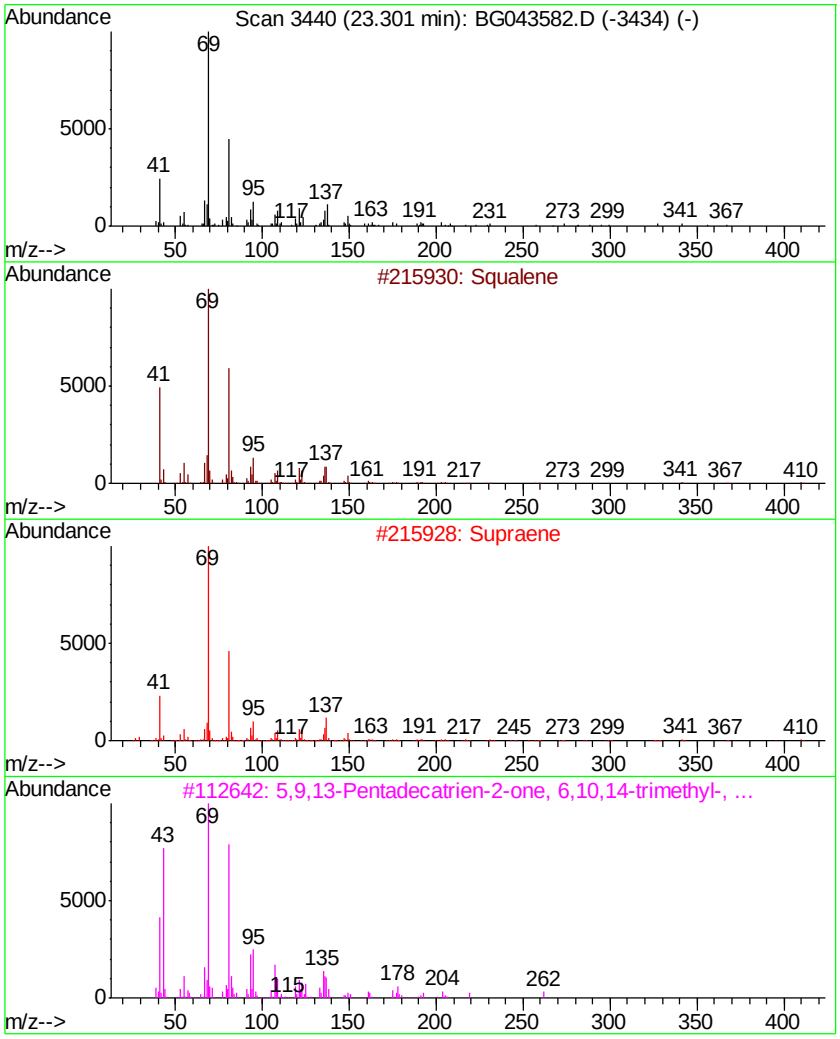
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

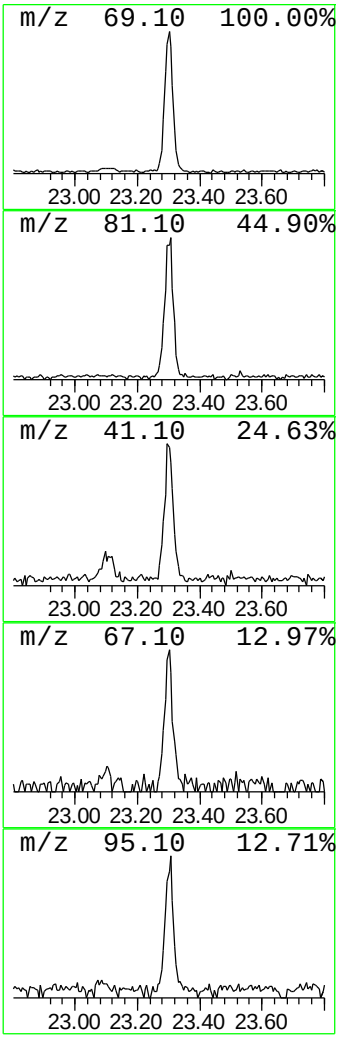
****

Peak Number 7 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.30	6.10 ng	174476	Perylene-d12	24.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	90
2	Supraene	410	C30H50	007683-64-9	90
3	5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	59
4	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	56
5	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	53





Tentatively Identified Compound (LSC) summary

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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...	3.17	19.5	ng	170250	1	8.00	174734	20.0
1,3,5-Cycloheptat...	4.18	56.2	ng	491123	1	8.00	174734	20.0
2-Pentanone, 4-hy...	5.11	18.6	ng	162267	1	8.00	174734	20.0
unknown7.55	7.55	109.4	ng	955529	1	8.00	174734	20.0
1-Dodecanol, 2-oc...	21.29	4.8	ng	127830	5	21.64	531905	20.0
Squalene	23.30	6.1	ng	174476	6	24.83	571904	20.0