LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG091215\
Data File : BG018658.D
Acq On : 12 Sep 2015 3:03
Operator : UM/IZ
Sample : G3637-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : VITALE-FILL-SOURCE-1B

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-BG091115.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	2.962	16	21	38	rVV	2975377	4099799	100.00%	15.251%
2	3.109	40	46	53	rBV2	42003	79192	1.93%	0.295%
3	3.179	53	58	77	rVB	605772	870423	21.23%	3.238%
4	5.107	380	386	397	rVB	389374	568288	13.86%	2.114%
5	5.577	459	466	479	rVB	883206	1351068	32.95%	5.026%
6	7.169	728	737	746	rBV	889774	1495893	36.49%	5.565%
7	7.539	792	800	815	rBV	884082	1479449	36.09%	5.503%
8	8.003	873	879	886	rBV	196722	334852	8.17%	1.246%
9	8.326	927	934	943	rVB	650347	1099902	26.83%	4.092%
10	9.161	1068	1076	1088	rBV	519205	910651	22.21%	3.388%
11	10.806	1349	1356	1364	rVB	270740	479345	11.69%	1.783%
12	13.256	1765	1773	1786	rBV	1494086	2245653	54.77%	8.354%
13	14.078	1907	1913	1920	rBV	312718	443573	10.82%	1.650%
14	14.631	2000	2007	2018	rBV2	460601	742697	18.12%	2.763%
15	16.117	2253	2260	2269	rBV	1341774	2031736	49.56%	7.558%
16	16.335	2292	2297	2300	rBV2	31652	48089	1.17%	0.179%
17	17.128	2427	2432	2435	rBV	34403	44877	1.09%	0.167%
18	17.375	2466	2474	2480	rBV2	692855	1054235	25.71%	3.922%
19	18.133	2598	2603	2614	rBV8	24243	57994	1.41%	0.216%
20	18.256	2620	2624	2634	rBV	224734	353896	8.63%	1.316%
21	19.525	2834	2840	2844	rBV4	41219	61748	1.51%	0.230%
22	19.983	2911	2918	2925	rBV	3083079	3898713	95.10%	14.503%
23	21.276	3134	3138	3148	rBV3	83282	170018	4.15%	0.632%
24	21.628	3192	3198	3205	rBV	814205	1311860	32.00%	4.880%
25	23.303	3477	3483	3490	rBV	198341	361501	8.82%	1.345%
26	24.819	3731	3741	3753	rBV2	461258	1286561	31.38%	4.786%

Sum of corrected areas: 26882013

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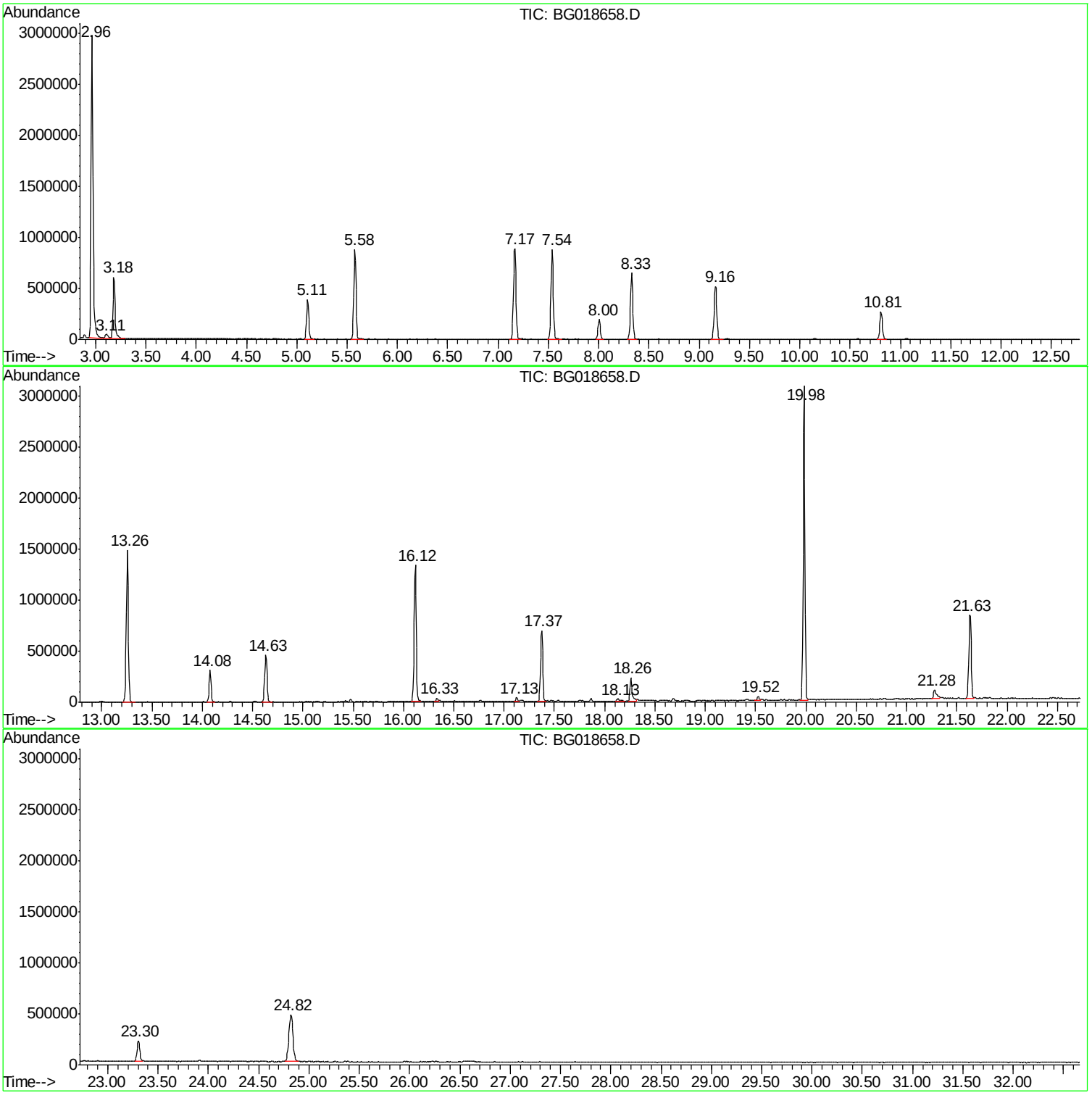
Instrument :
BNA_G
ClientSampleId :
VITALE-FILL-SOURCE-1B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG091215\
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Operator : UM/IZ
Sample : G3637-02
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ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VITALE-FILL-SOURCE-1B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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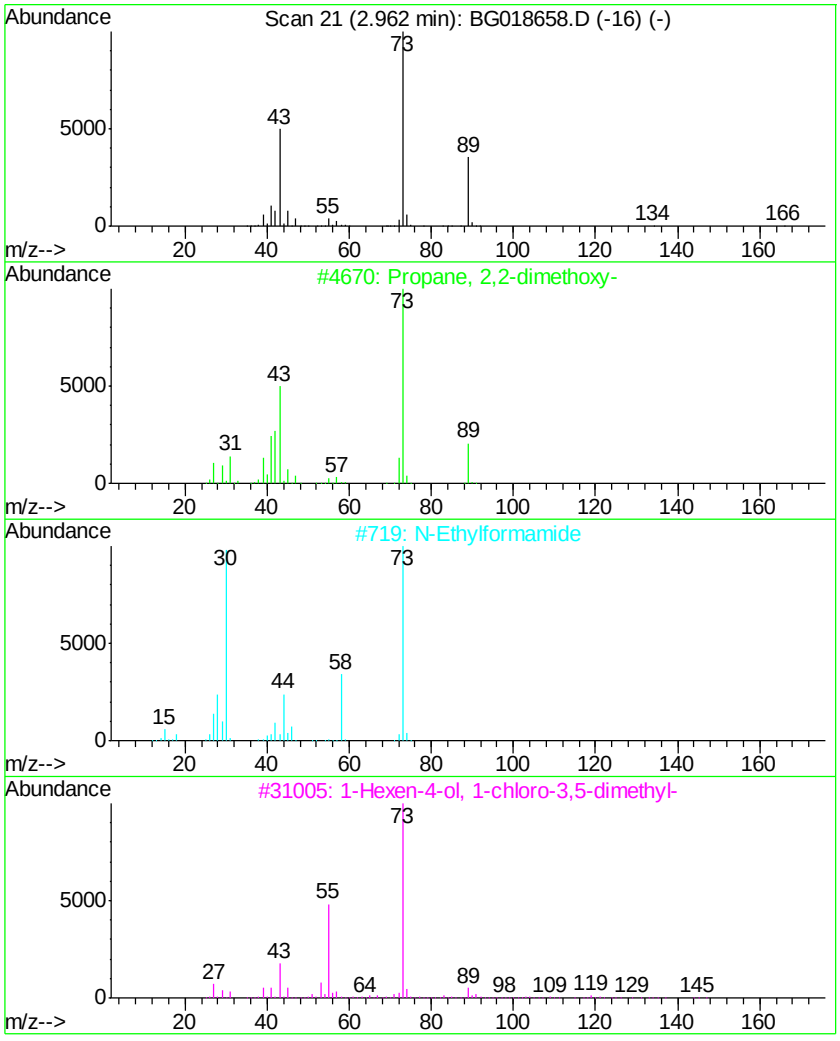
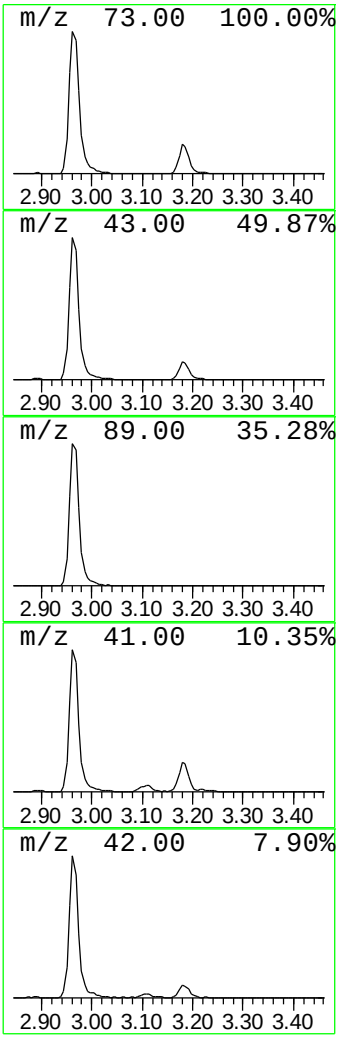
Peak Number 1 unknown2.96 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.96	244.87 ng	4099800	1,4-Dichlorobenzene-d4	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5	1-Propene-1-thiol	74	C3H6S	000925-89-3	7





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Operator : UM/IZ
Sample : G3637-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VITALE-FILL-SOURCE-1B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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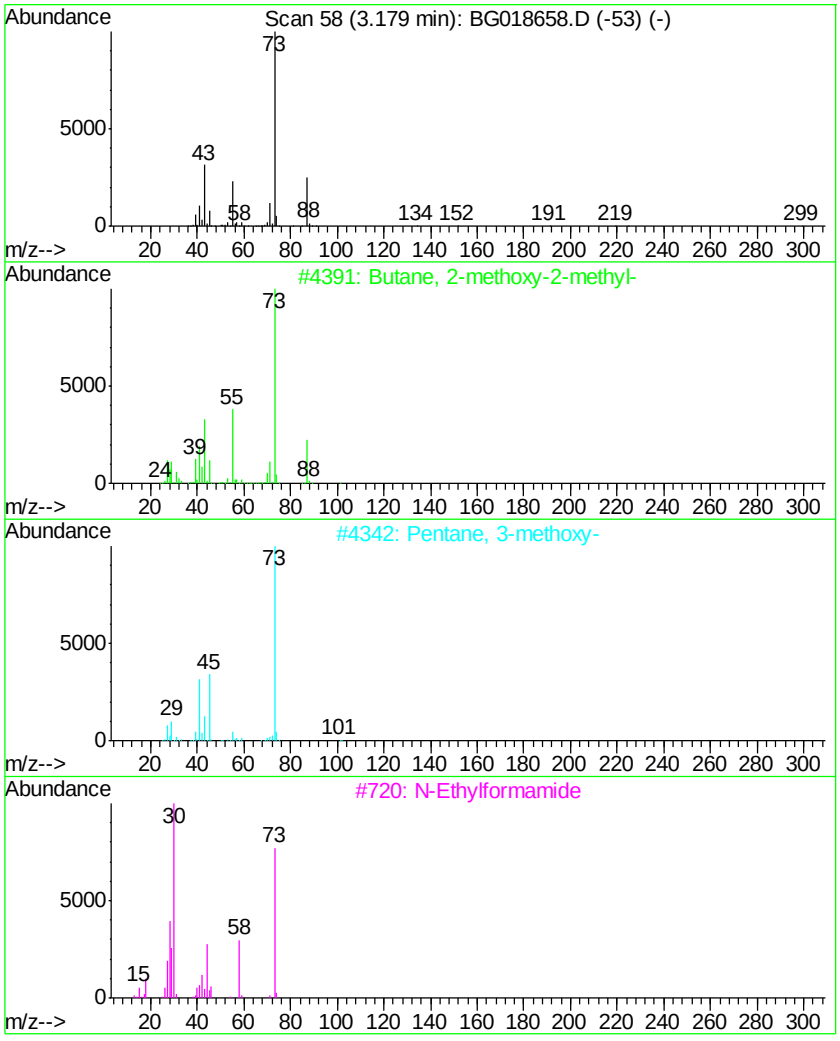
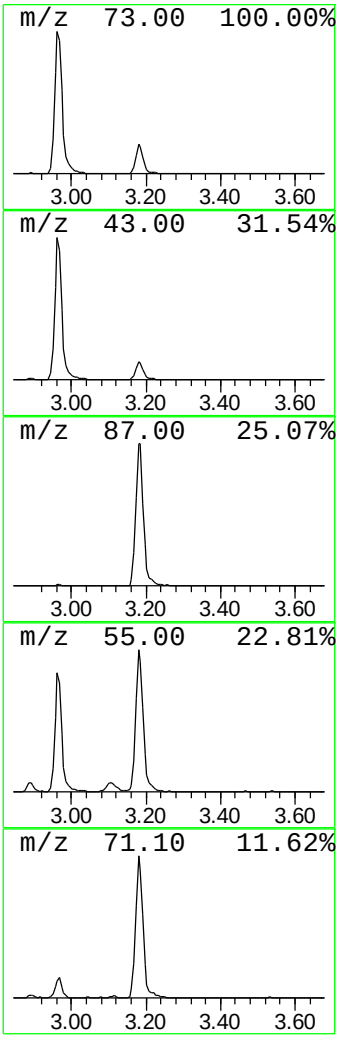
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	51.99 ng	870423	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	83
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG091215\
Data File : BG018658.D
Acq On : 12 Sep 2015 3:03
Operator : UM/IZ
Sample : G3637-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VITALE-FILL-SOURCE-1B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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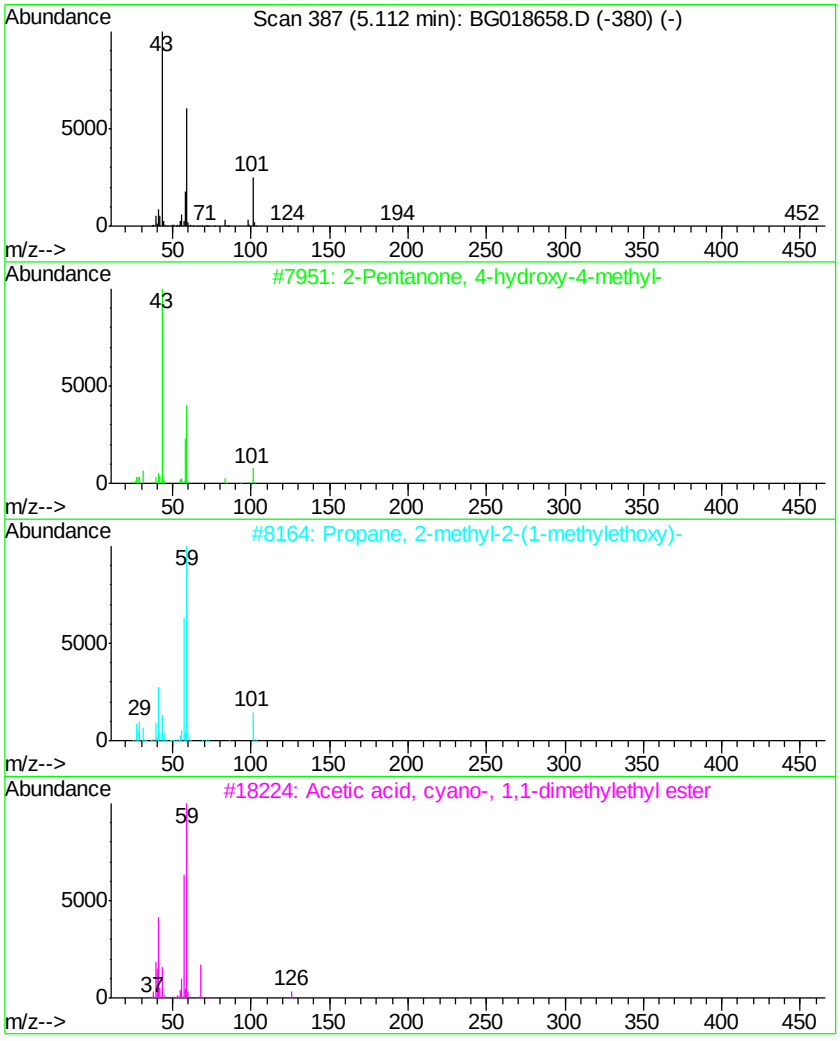
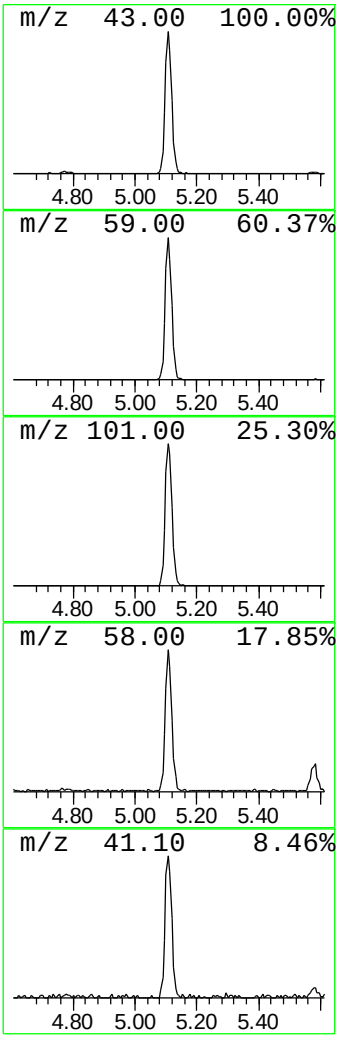
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	33.94 ng	568288	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	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	50
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23
5	Acetone	58	C3H6O	000067-64-1	10





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Operator : UM/IZ
Sample : G3637-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VITALE-FILL-SOURCE-1B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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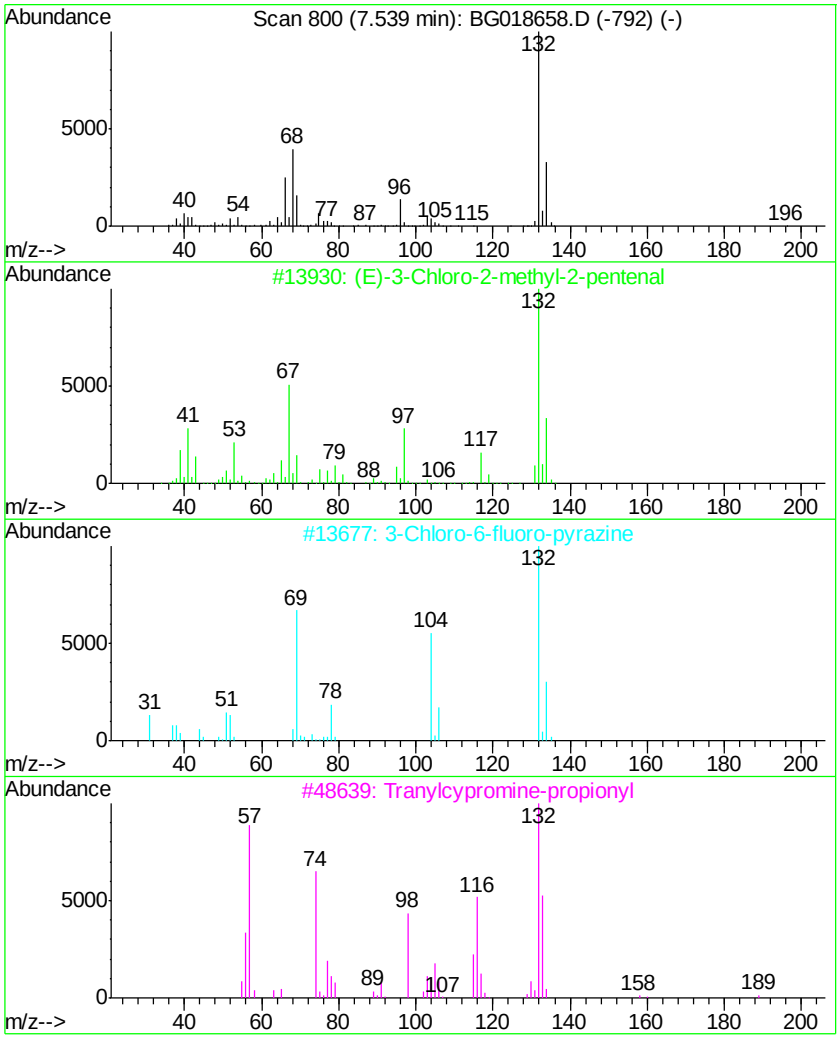
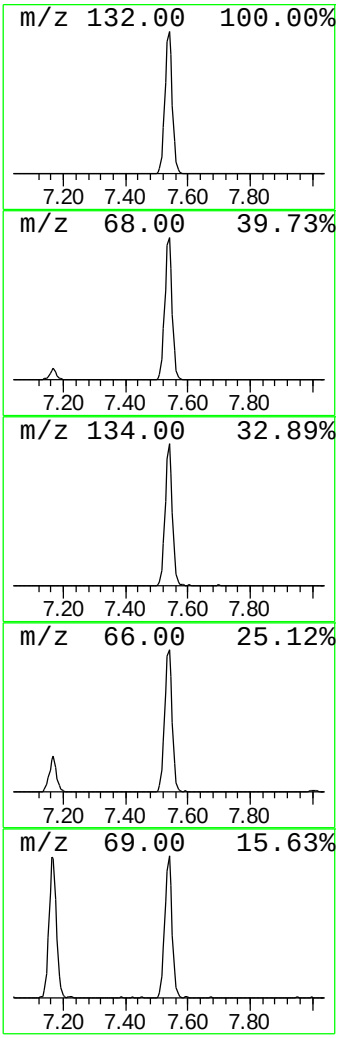
Peak Number 5 unknown7.54 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.54	88.36 ng	1479450	1,4-Dichlorobenzene-d4	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Operator : UM/IZ
Sample : G3637-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VITALE-FILL-SOURCE-1B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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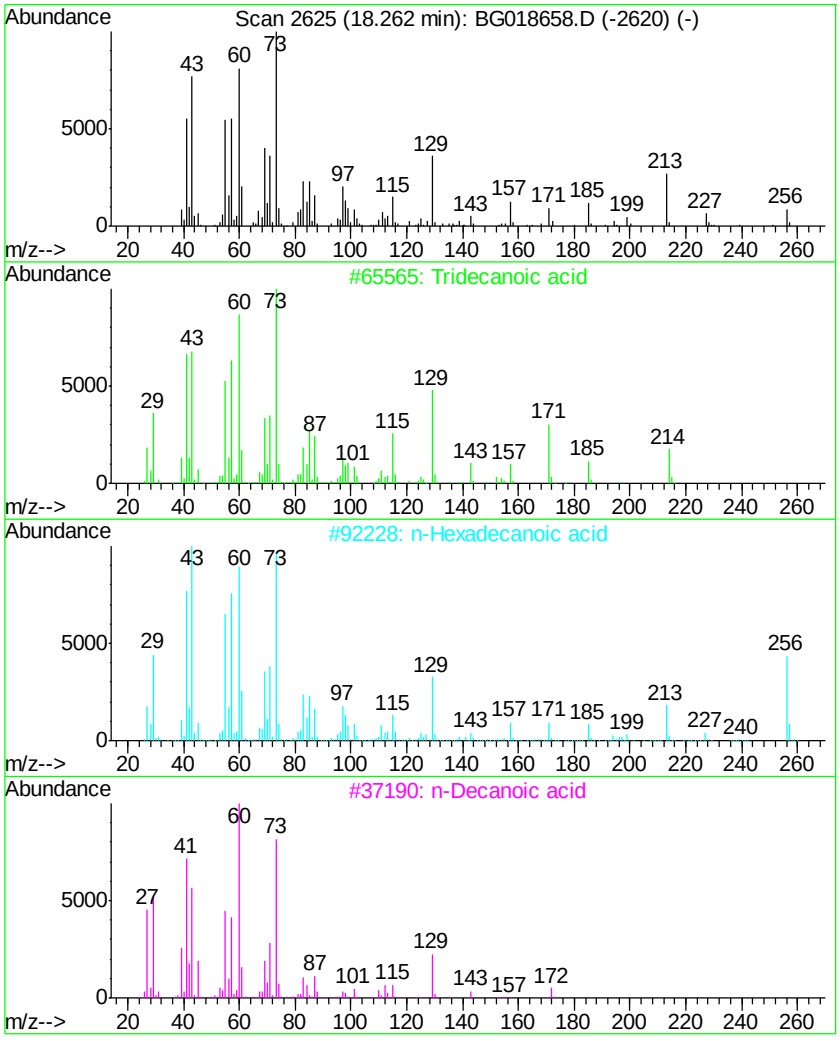
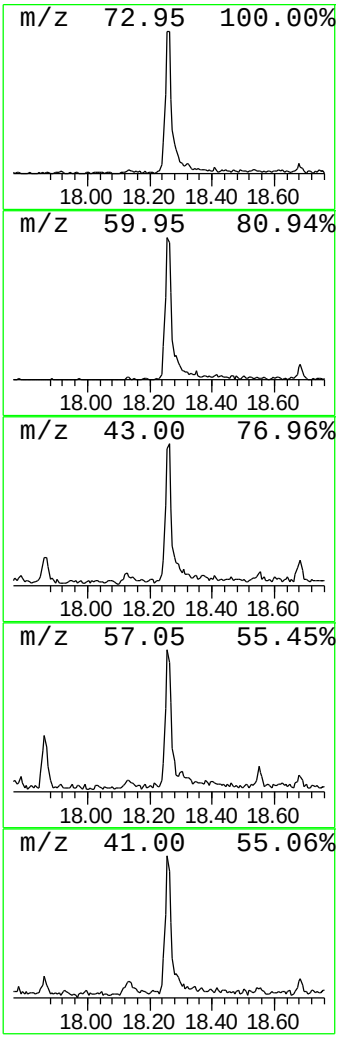
Peak Number 7 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.26	6.71 ng	353896	Phenanthrene-d10	17.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	94
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
3	n-Decanoic acid	172	C10H20O2	000334-48-5	62
4	Amyl Nitrite	117	C5H11NO2	000110-46-3	14
5	Hexadecane	226	C16H34	000544-76-3	11





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Sample : G3637-02
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ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VITALE-FILL-SOURCE-1B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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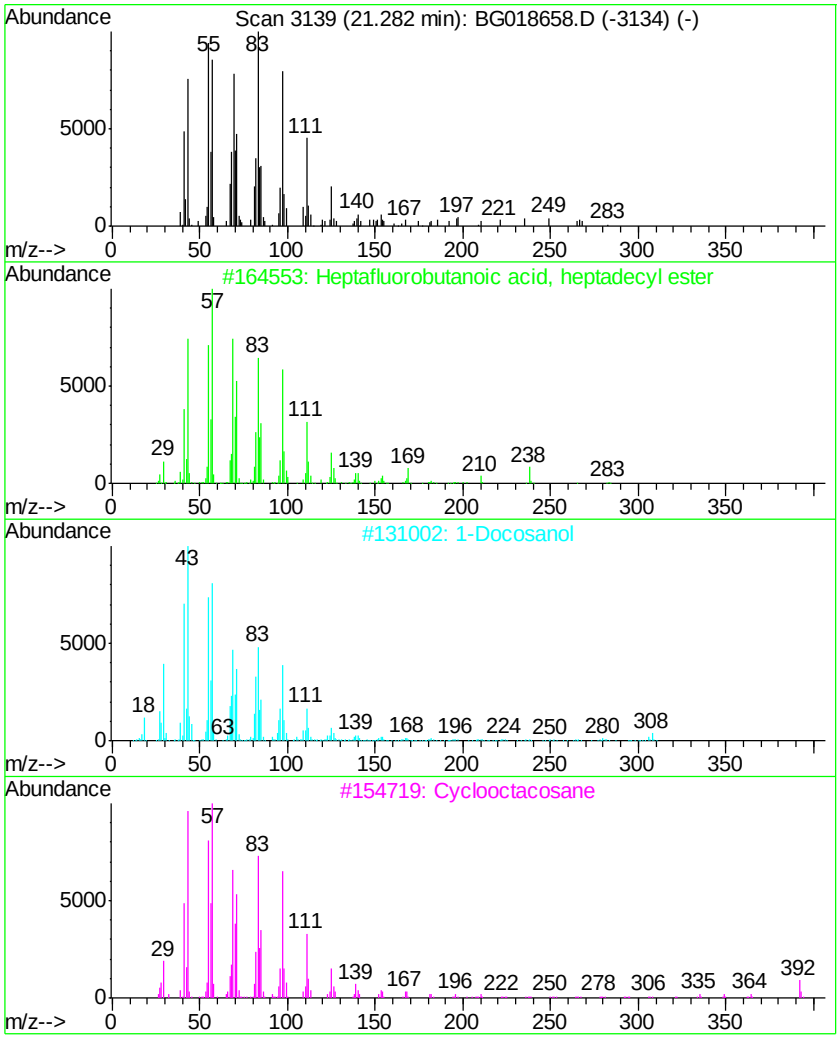
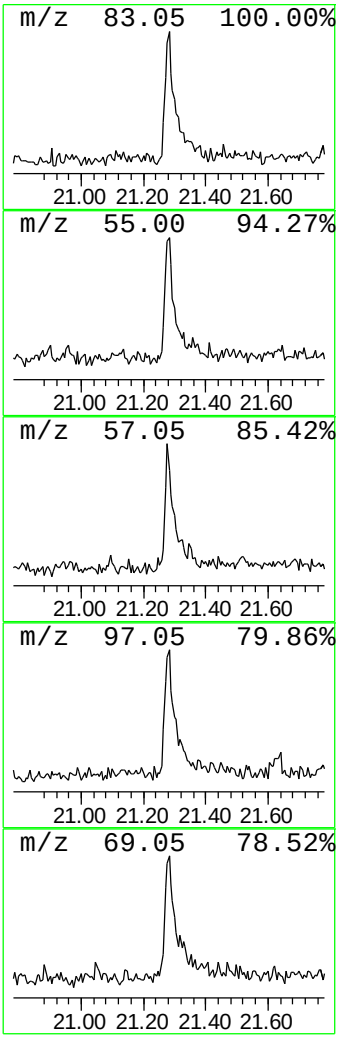
Peak Number 8 Heptafluorobutanoic acid, h... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.28	2.59 ng	170018	Chrysene-d12	21.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	91
2	1-Docosanol	326	C22H46O	000661-19-8	91
3	Cyclooctacosane	392	C28H56	000297-24-5	90
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
5	1-Tricosene	322	C23H46	018835-32-0	90





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Instrument : BNA_G
ClientSampleId : VITALE-FILL-SOURCE-1B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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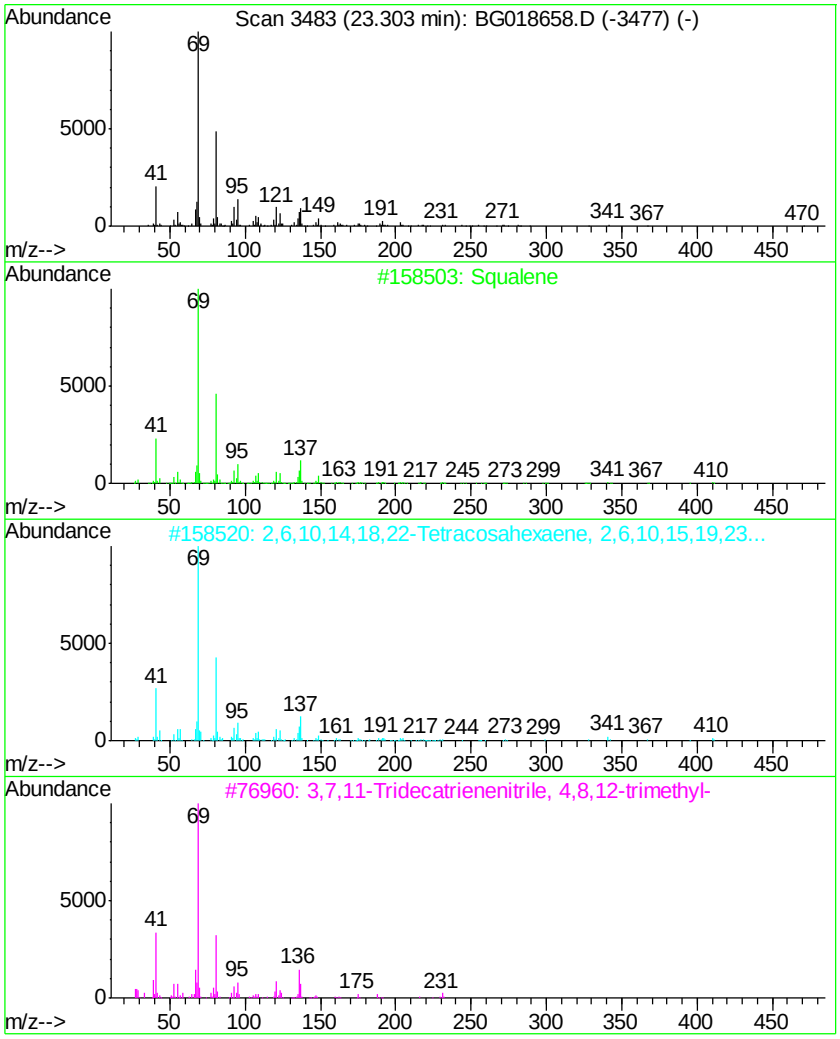
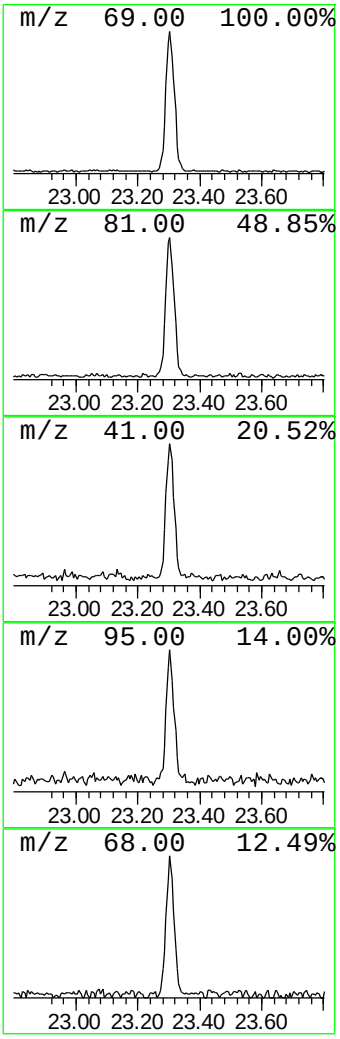
Peak Number 9 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.30	5.62 ng	361501	Perylene-d12	24.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	91
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	87
3	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	78
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5	3,7,11-Tridecatrienoic acid, 4,8...	264	C17H28O2	036237-69-1	64





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown2.96	2.96	244.9	ng	4099800	1	8.00	334852	20.0
Butane, 2-methoxy...	3.18	52.0	ng	870423	1	8.00	334852	20.0
2-Pentanone, 4-hy...	5.11	33.9	ng	568288	1	8.00	334852	20.0
unknown7.54	7.54	88.4	ng	1479450	1	8.00	334852	20.0
Tridecanoic acid	18.26	6.7	ng	353896	4	17.37	1054240	20.0
Heptafluorobutano...	21.28	2.6	ng	170018	5	21.63	1311860	20.0
Squalene	23.30	5.6	ng	361501	6	24.82	1286560	20.0