LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033258.D
Acq On : 20 Mar 2018 2:37
Operator : SJ/JU
Sample : J1953-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-JETT-E-U-M

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-BG031918.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	3.499	30	36	46	rBV	138241	273556	4.20%	1.209%
2	3.587	46	51	60	rVB	85831	140041	2.15%	0.619%
3	6.313	509	515	533	rBV	131599	337623	5.19%	1.492%
4	6.866	599	609	635	rBV	2862747	6507326	100.00%	28.756%
5	8.000	795	802	814	rBV2	74979	221357	3.40%	0.978%
6	8.405	862	871	888	rBV	312568	728820	11.20%	3.221%
7	8.893	948	954	967	rBV2	96172	233130	3.58%	1.030%
8	9.228	1003	1011	1028	rBV	497452	1014217	15.59%	4.482%
9	10.091	1149	1158	1180	rBV	400274	945034	14.52%	4.176%
10	11.777	1438	1445	1457	rBV	153277	334212	5.14%	1.477%
11	14.139	1840	1847	1861	rBV	1287402	2271523	34.91%	10.038%
12	15.508	2074	2080	2093	rVB2	305054	529343	8.13%	2.339%
13	16.983	2324	2331	2343	rBV	835610	1421503	21.84%	6.282%
14	17.124	2352	2355	2364	rVB2	38082	69584	1.07%	0.307%
15	18.241	2535	2545	2557	rBV	449621	795891	12.23%	3.517%
16	19.034	2676	2680	2690	rBV2	100113	170700	2.62%	0.754%
17	20.156	2863	2871	2880	rBV6	73023	182486	2.80%	0.806%
18	20.268	2886	2890	2898	rBV3	54959	74951	1.15%	0.331%
19	20.761	2968	2974	2985	rBV	2710650	3738284	57.45%	16.519%
20	22.107	3198	3203	3209	rBV2	104018	182388	2.80%	0.806%
21	22.389	3247	3251	3257	rVB	112011	174660	2.68%	0.772%
22	22.594	3278	3286	3298	rBV2	445345	868725	13.35%	3.839%
23	23.887	3499	3506	3515	rVB	297552	587386	9.03%	2.596%
24	26.384	3921	3931	3951	rVB2	235349	826940	12.71%	3.654%

Sum of corrected areas: 22629680

LSC Report - Integrated Chromatogram

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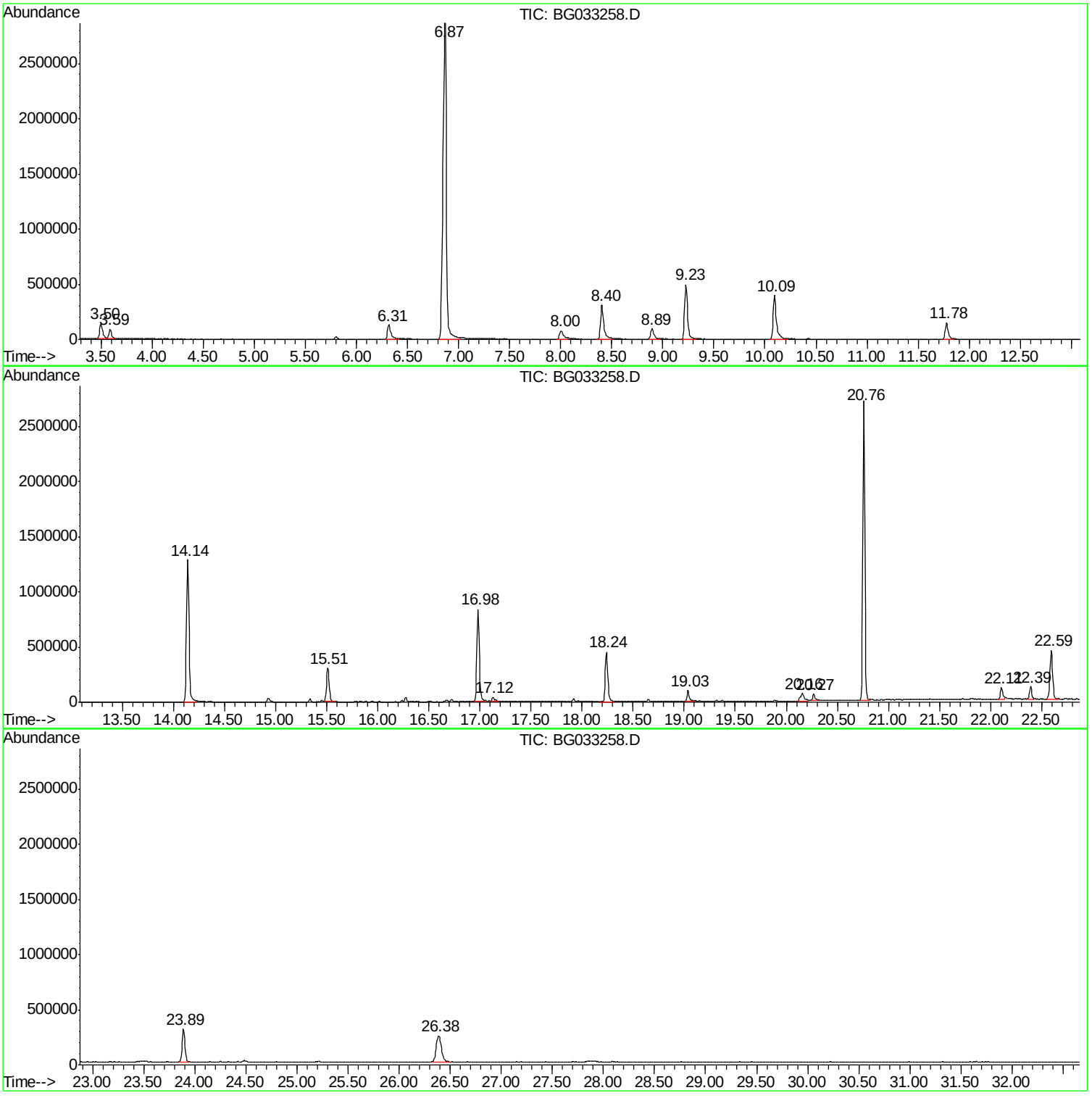
Instrument : BNA_G
ClientSampleId : 031418-JETT-E-U-M

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
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Misc :
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ClientSampleId : 031418-JETT-E-U-M

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

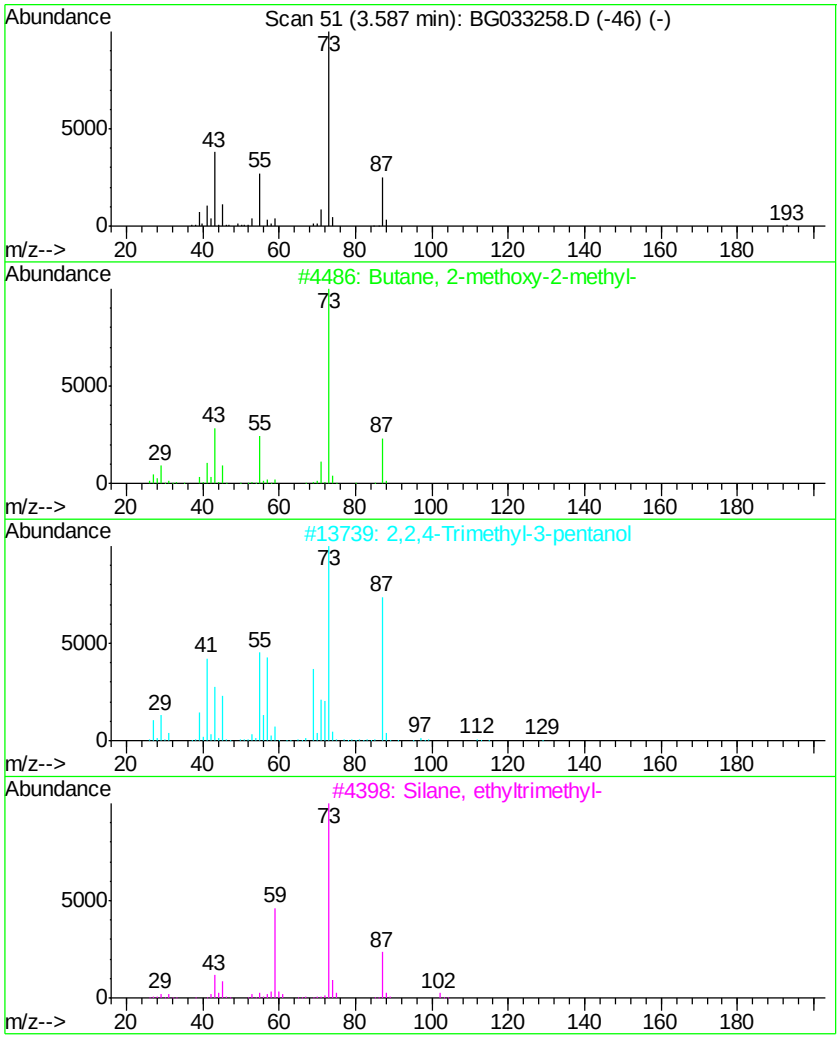
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

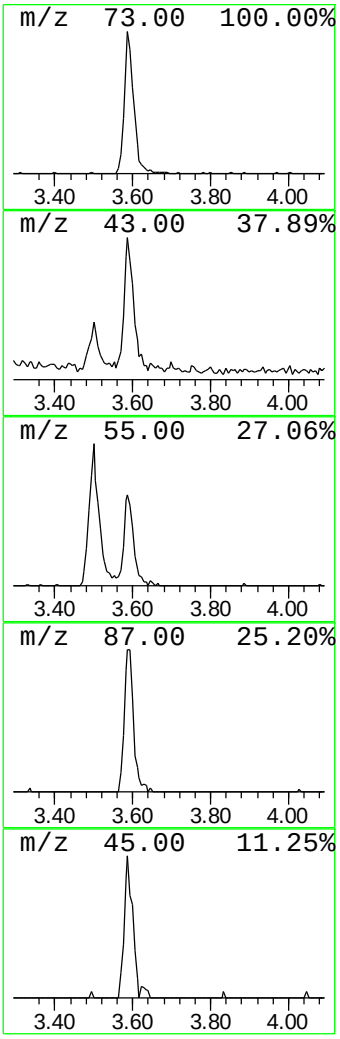
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.59	12.01 ng	140041	1,4-Dichlorobenzene-d4	8.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	33
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





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Acq On : 20 Mar 2018 2:37
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Sample : J1953-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-JETT-E-U-M

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

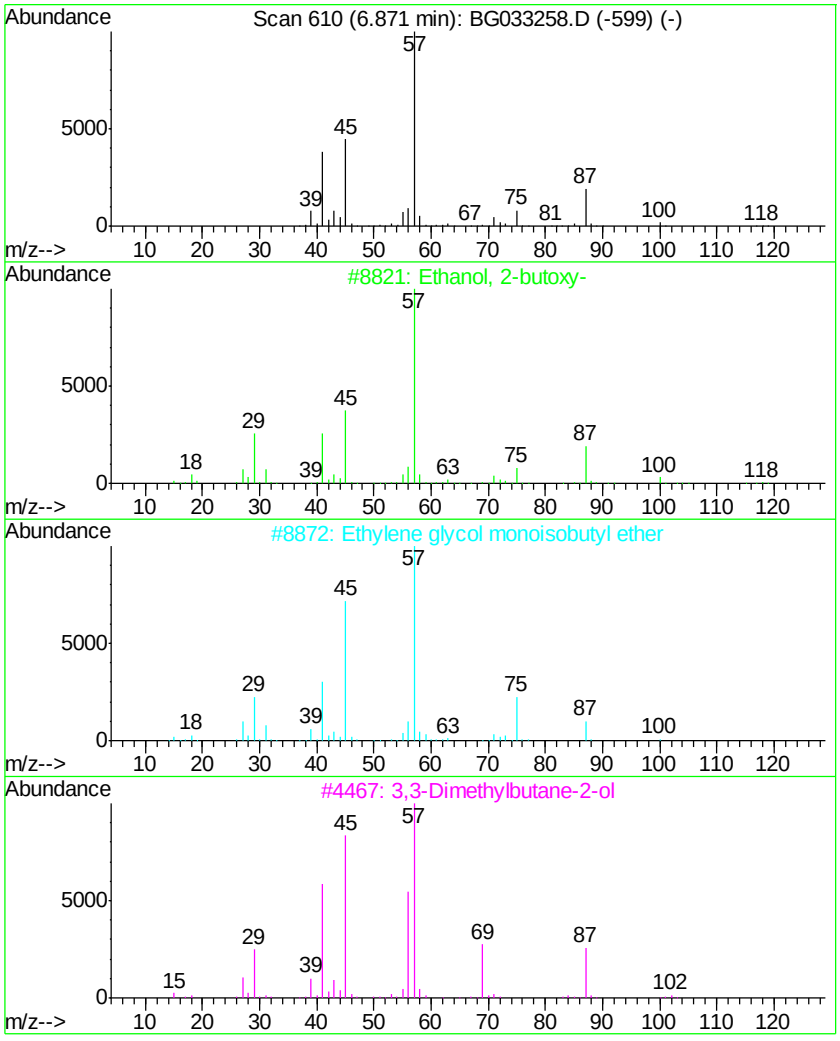
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

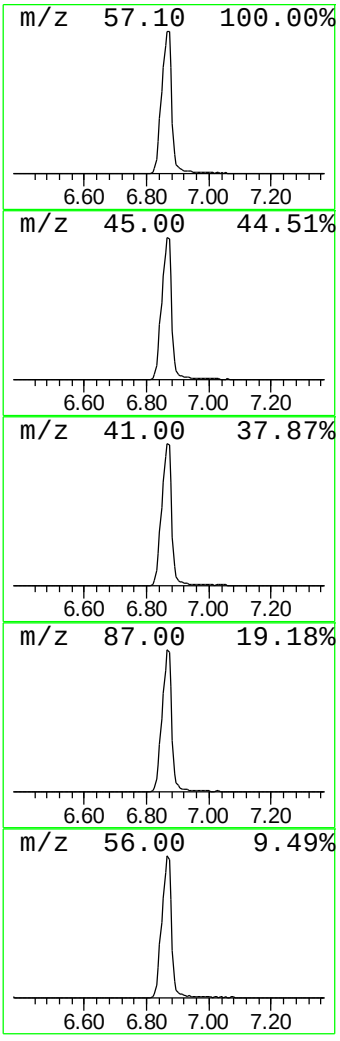
****

Peak Number 3 Ethanol, 2-butoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.87	558.26 ng	6507330	1,4-Dichlorobenzene-d4	8.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	78
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	53
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	42
4	Formic acid, 3,3-dimethylbut-2-y...	130	C7H14O2	1000368-20-5	39
5	n-Butyl ether	130	C8H18O	000142-96-1	25





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Data File : BG033258.D
Acq On : 20 Mar 2018 2:37
Operator : SJ/JU
Sample : J1953-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-JETT-E-U-M

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

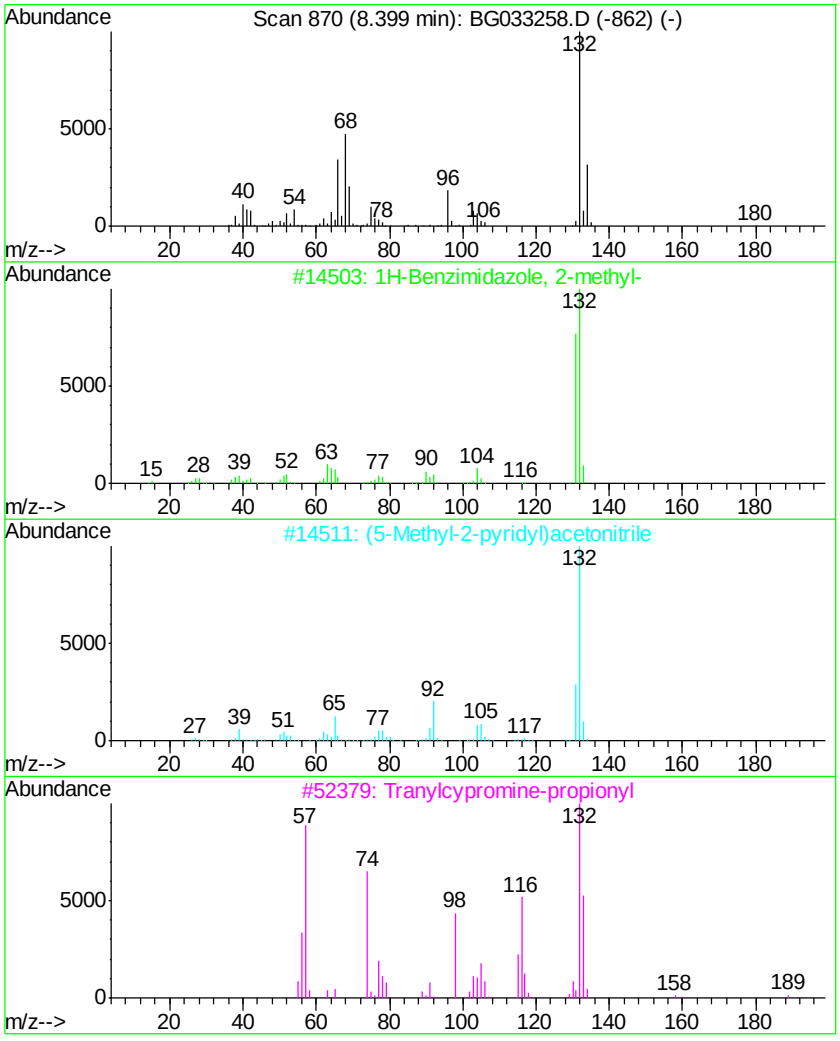
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

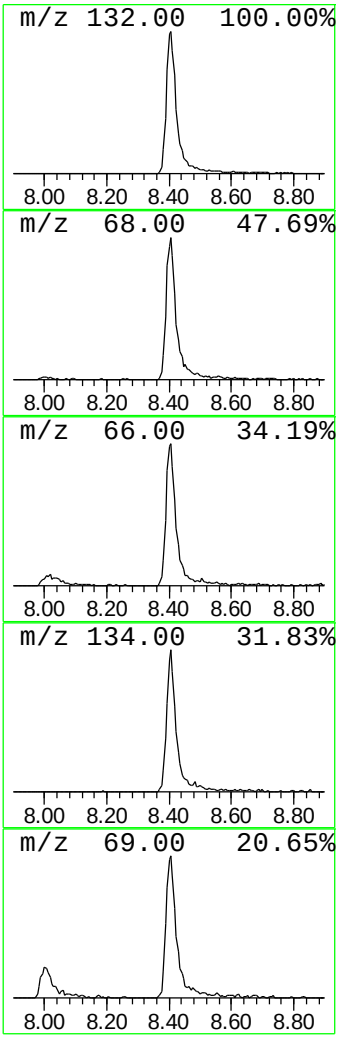
****

Peak Number 4 unknown8.40 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.40	62.52 ng	728820	1,4-Dichlorobenzene-d4	8.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	25
2	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	22
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





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Data File : BG033258.D
Acq On : 20 Mar 2018 2:37
Operator : SJ/JU
Sample : J1953-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-JETT-E-U-M

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

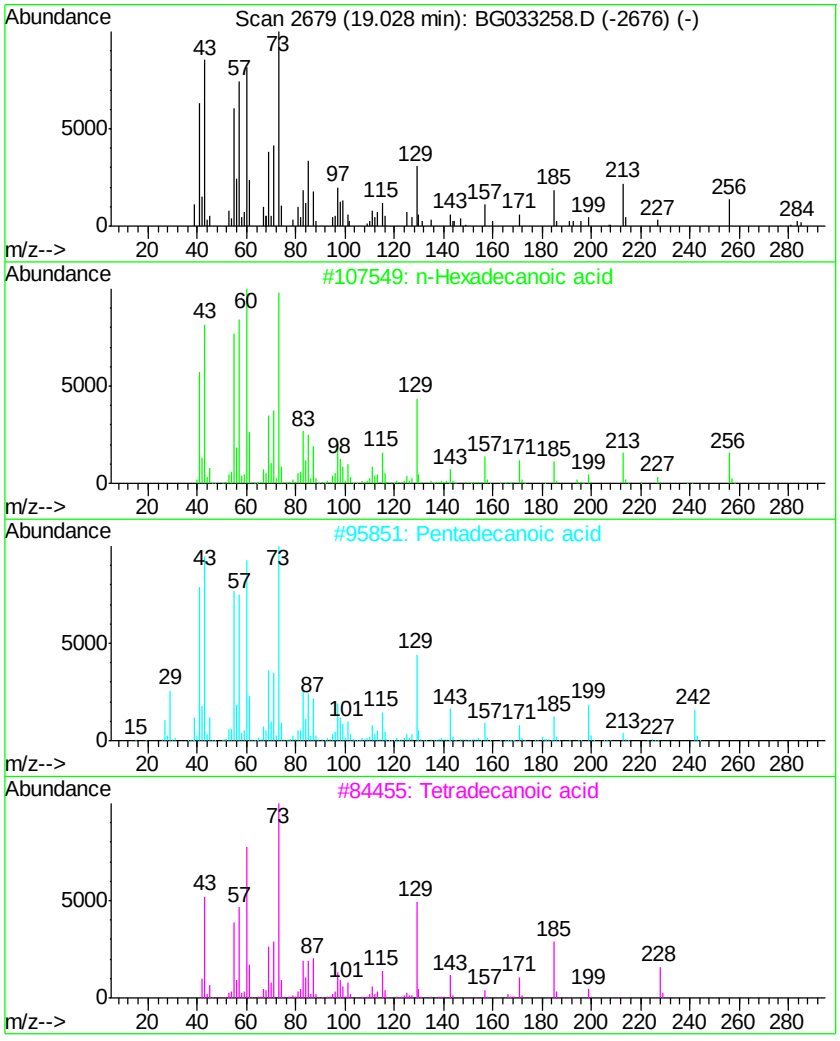
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

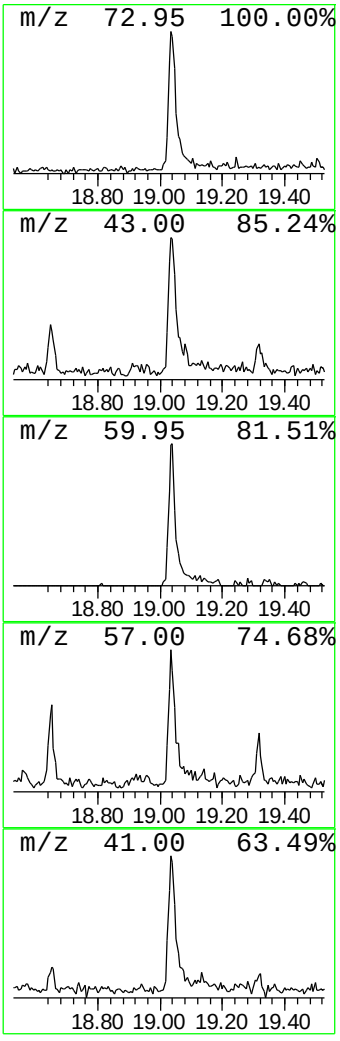
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.03	4.29 ng	170700	Phenanthrene-d10	18.24

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	76
4	n-Decanoic acid	172	C10H20O2	000334-48-5	47
5	Eicosane	282	C20H42	000112-95-8	25





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033258.D
Acq On : 20 Mar 2018 2:37
Operator : SJ/JU
Sample : J1953-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-JETT-E-U-M

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

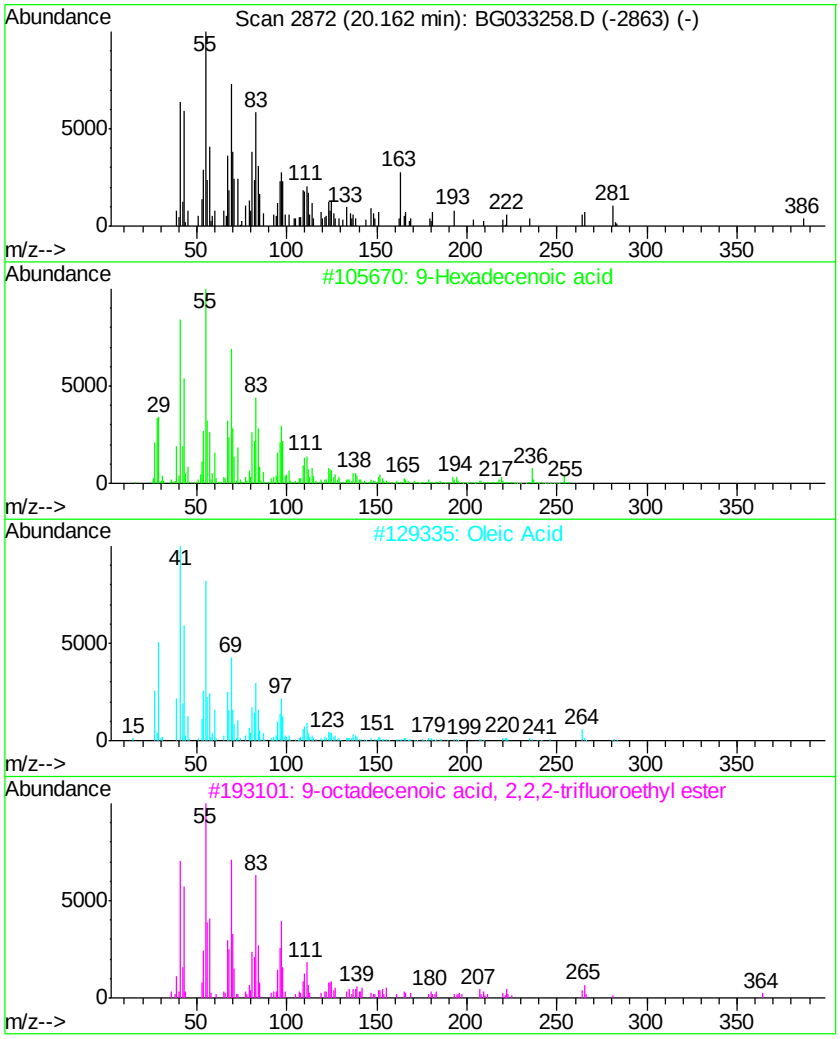
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

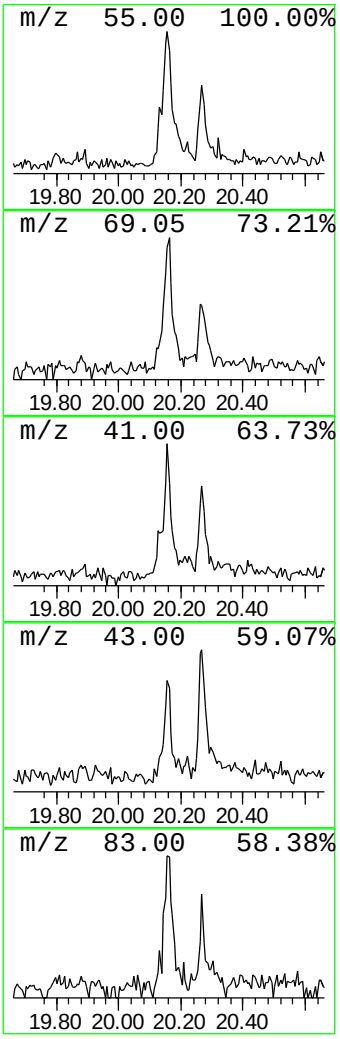
****

Peak Number 7 9-Hexadecenoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.16	4.59 ng	182486	Phenanthrene-d10	18.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Hexadecenoic acid	254	C16H30O2	002091-29-4	87
2	Oleic Acid	282	C18H34O2	000112-80-1	86
3	9-octadecenoic acid, 2,2,2-trifl...	364	C20H35F3O2	1000376-54-3	76
4	Octadec-9-enoic acid	282	C18H34O2	1000190-13-7	74
5	cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1000333-58-3	62





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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-JETT-E-U-M

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

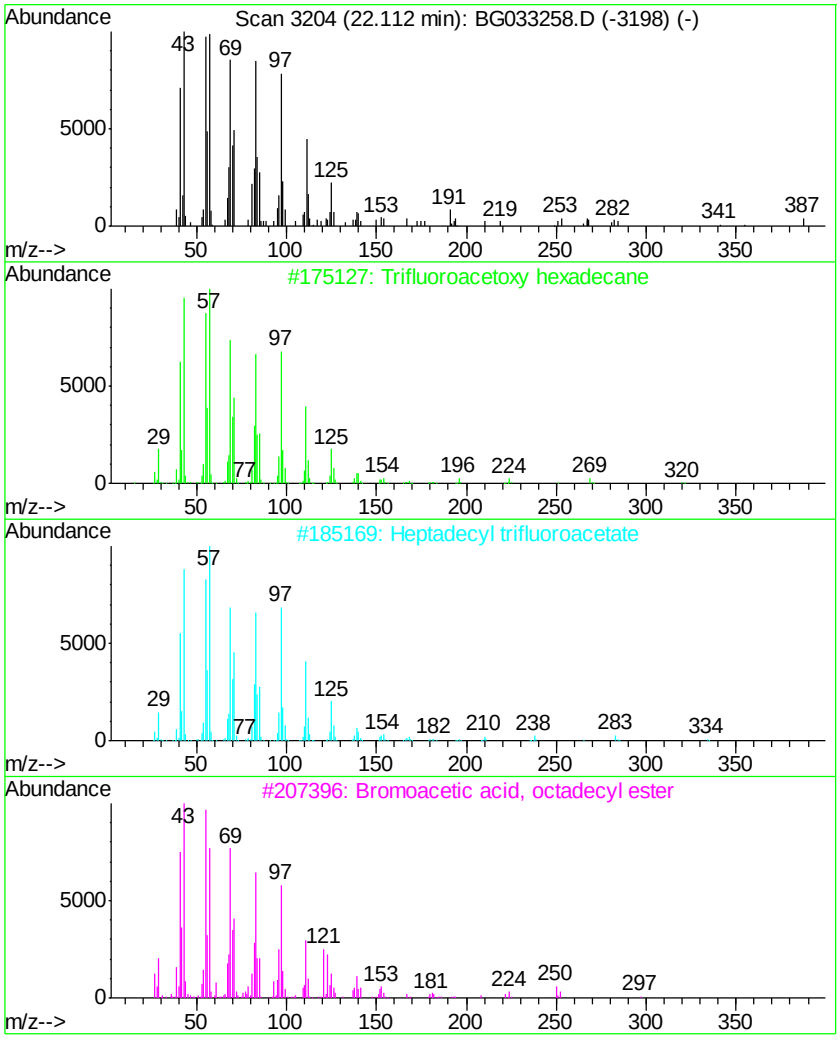
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

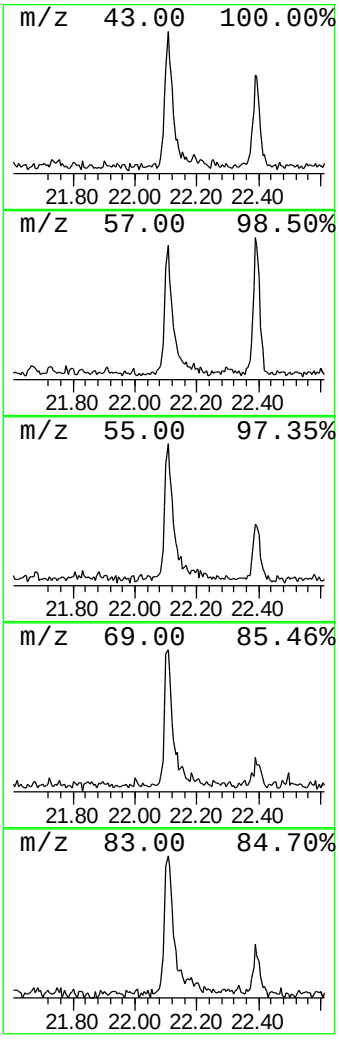
****

Peak Number 8 Trifluoroacetoxy hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.11	4.20 ng	182388	Chrysene-d12	22.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
3	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	90
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90





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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

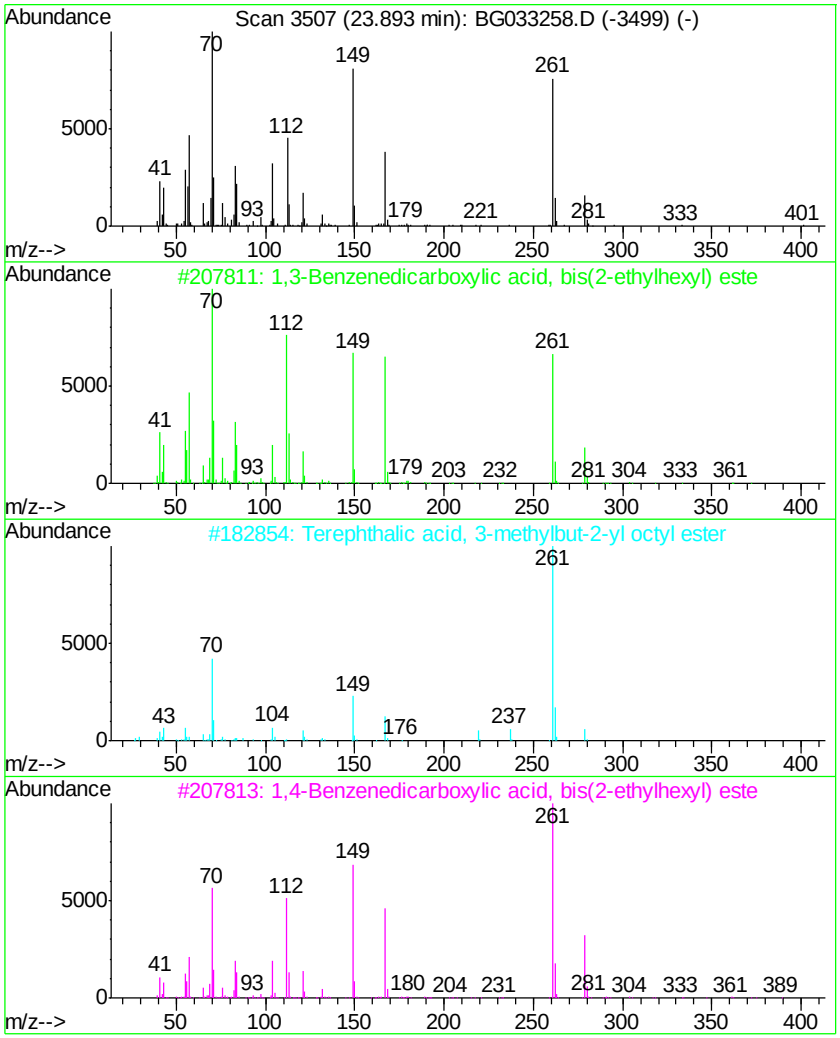
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

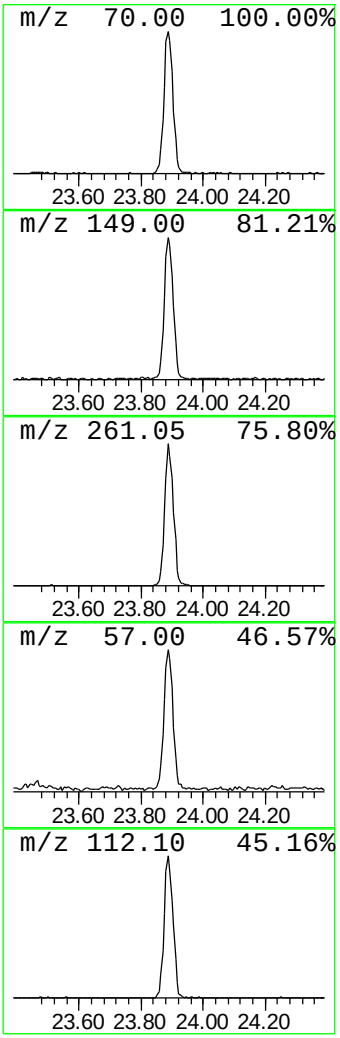
****

Peak Number 9 1,3-Benzenedicarboxylic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.89	13.52 ng	587386	Chrysene-d12	22.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	64
2	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	64
3	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	52
4	Isophthalic acid, octyl undec-2-...	430	C27H42O4	1000343-91-0	38
5	Phthalic acid, 3,5-difluoropheny...	320	C17H14F2O4	1000315-56-3	35





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...	3.59	12.0	ng	140041	1	8.89	233130	20.0
Ethanol, 2-butoxy-	6.87	558.3	ng	6507330	1	8.89	233130	20.0
unknown8.40	8.40	62.5	ng	728820	1	8.89	233130	20.0
n-Hexadecanoic acid	19.03	4.3	ng	170700	4	18.24	795891	20.0
9-Hexadecenoic acid	20.16	4.6	ng	182486	4	18.24	795891	20.0
Trifluoroacetoxy ...	22.11	4.2	ng	182388	5	22.59	868725	20.0
1,3-Benzenedicarb...	23.89	13.5	ng	587386	5	22.59	868725	20.0