LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031521\
Data File : BM029142.D
Acq On : 15 Mar 2021 22:28
Operator : CG/JU
Sample : M1666-05 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : COMP-89-90

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_M\Methods\8270-BM022321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029142.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.857	125	148	159	rBB	24607	118935	2.10%	1.254%
2	5.763	455	472	476	rBV	1931586	5676913	100.00%	59.873%
3	6.904	630	666	669	rBV2	53916	338770	5.97%	3.573%
4	9.116	1011	1042	1046	rBV2	89118	469718	8.27%	4.954%
5	9.939	1151	1182	1193	rBB3	101015	461771	8.13%	4.870%
6	10.404	1256	1261	1267	rVB	45879	68691	1.21%	0.724%
7	13.680	1811	1818	1822	rVB2	42527	68818	1.21%	0.726%
8	14.092	1884	1888	1897	rVB	65734	109268	1.92%	1.152%
9	14.286	1917	1921	1923	rBV2	57845	81269	1.43%	0.857%
10	14.804	2005	2009	2015	rBV2	51715	77157	1.36%	0.814%
11	14.921	2023	2029	2034	rBV6	34663	82172	1.45%	0.867%
12	15.062	2048	2053	2059	rBV2	97775	158815	2.80%	1.675%
13	15.333	2094	2099	2105	rBV5	43329	123361	2.17%	1.301%
14	15.551	2132	2136	2141	rVB	76710	122127	2.15%	1.288%
15	16.027	2210	2217	2221	rBV2	233978	455134	8.02%	4.800%
16	16.586	2309	2312	2314	rBV	54318	75144	1.32%	0.793%
17	16.845	2352	2356	2369	rVB	274531	462200	8.14%	4.875%
18	17.045	2386	2390	2394	rBV3	118158	183699	3.24%	1.937%
19	21.127	3082	3084	3089	rVB	57106	67053	1.18%	0.707%
20	21.221	3097	3100	3105	rVB	111667	138549	2.44%	1.461%
21	23.356	3459	3463	3472	rVB2	77912	141979	2.50%	1.497%

Sum of corrected areas: 9481543

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Instrument :
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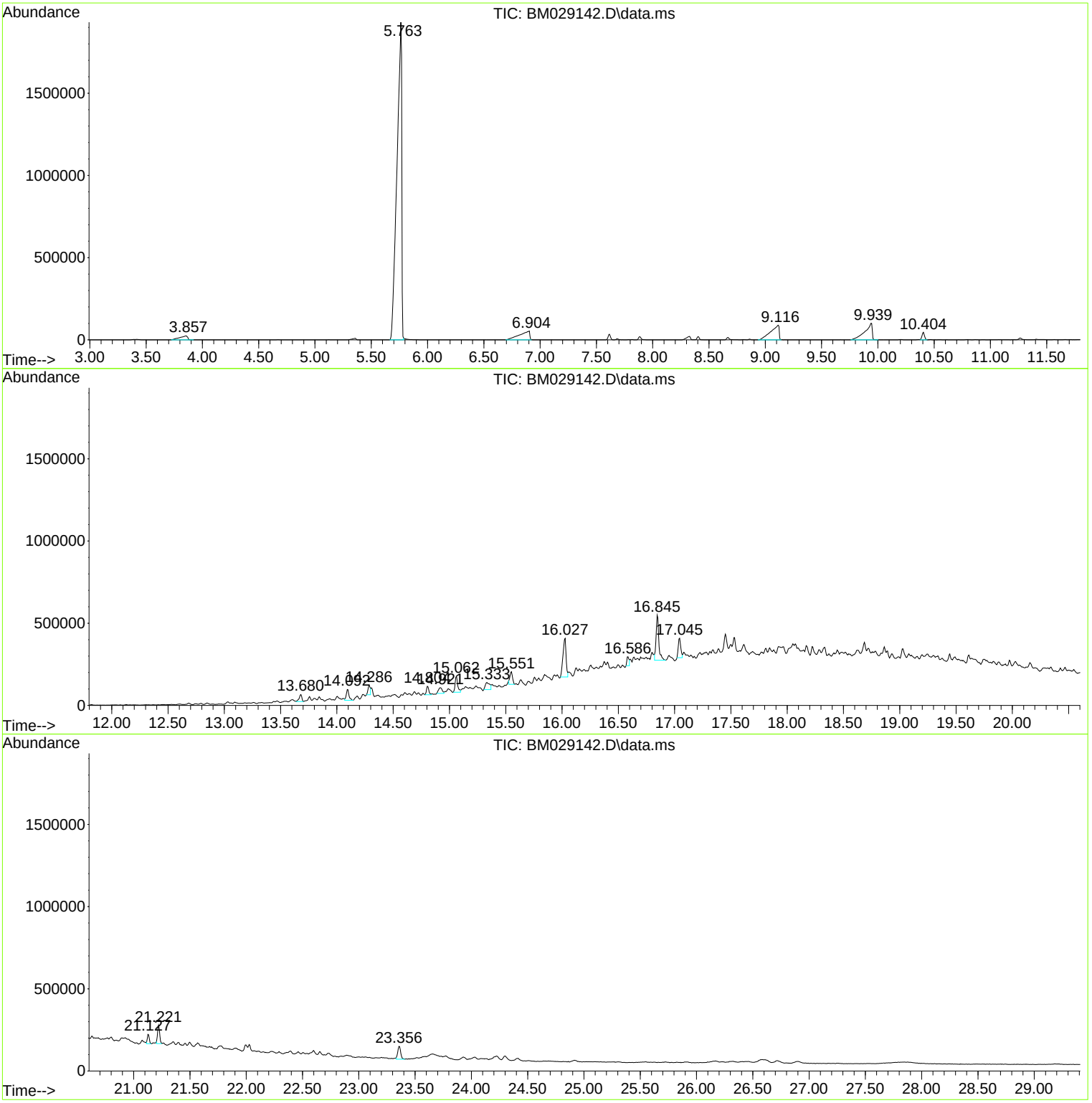
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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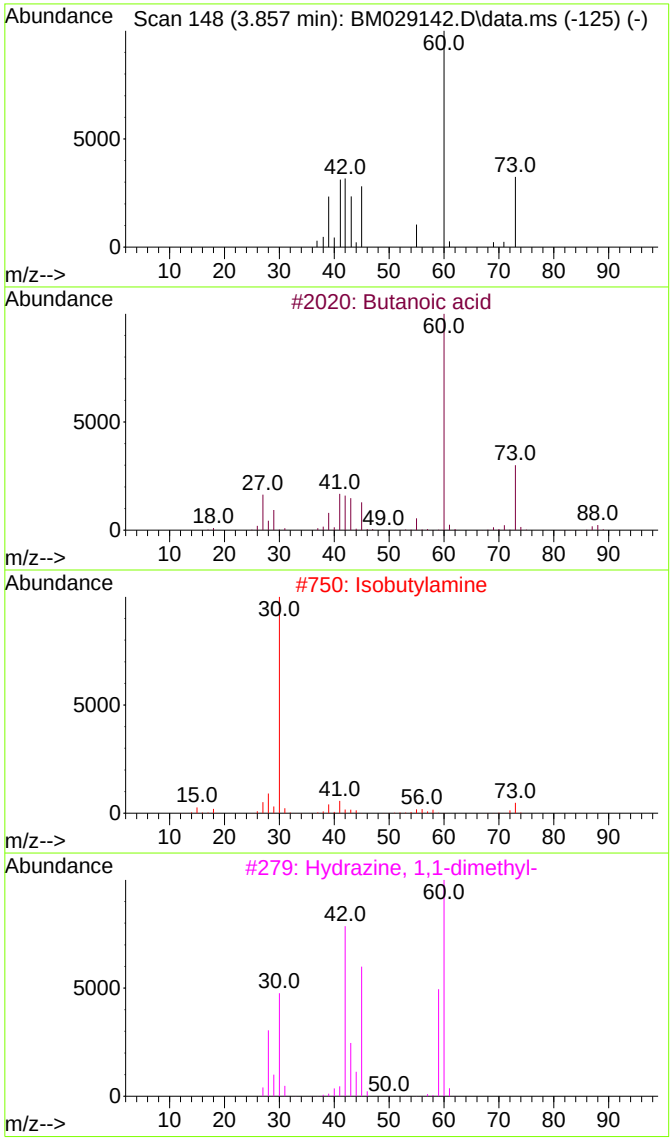
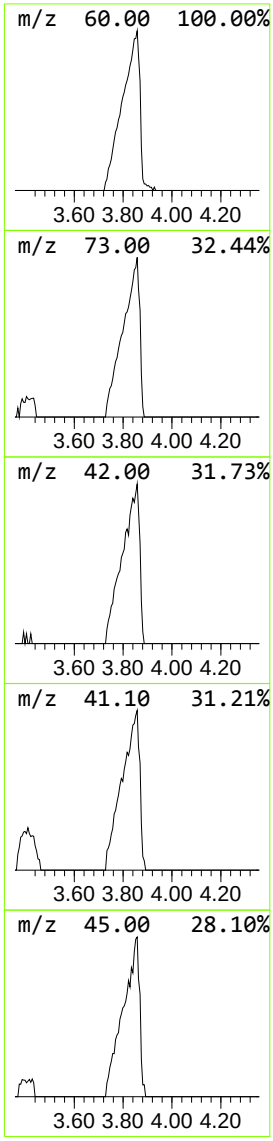
****
Peak Number 1 unknown3.857 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.857	7.02 ng	118935	1,4-Dichlorobenzene-d4	7.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid	88	C4H8O2	000107-92-6	39
2	Isobutylamine	73	C4H11N	000078-81-9	9
3	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	7
4	Carbonyl sulfide	60	COS	000463-58-1	5
5	Urea	60	CH4N2O	000057-13-6	5





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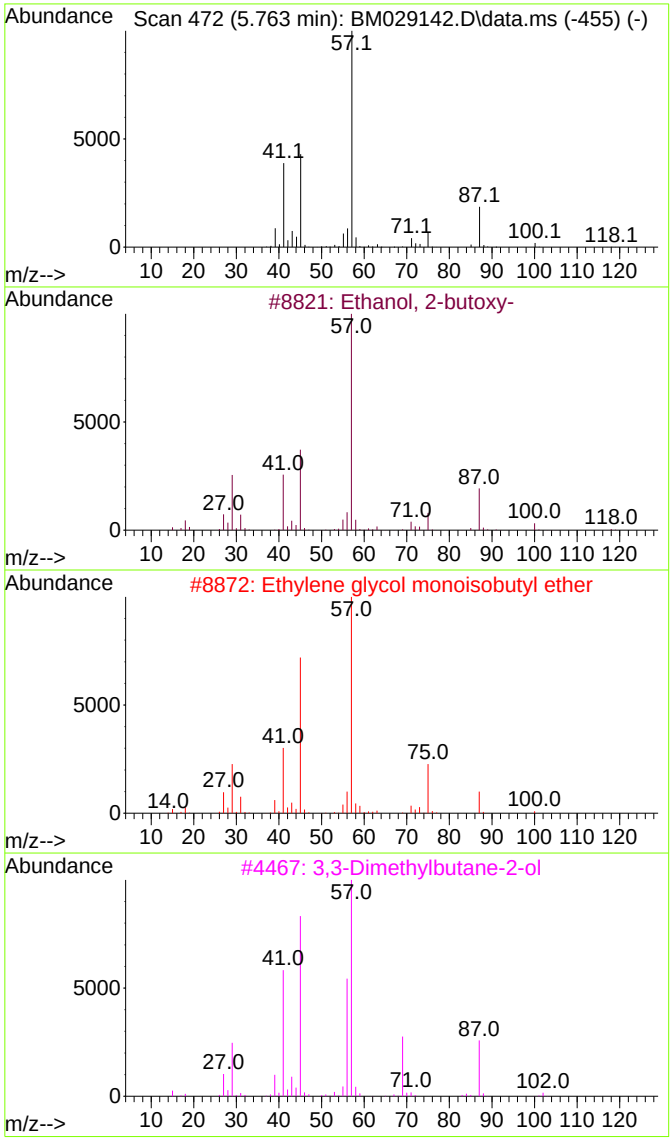
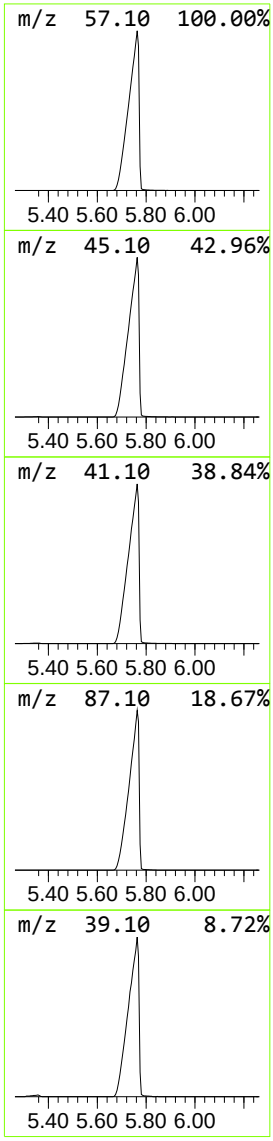
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.763	335.15 ng	5676910	1,4-Dichlorobenzene-d4	7.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	91
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	40
4	Formic acid, 3,3-dimethylbut-2-y...	130	C7H14O2	1000368-20-5	17
5	Propanoic acid, 2-methylpropyl e...	130	C7H14O2	000540-42-1	12





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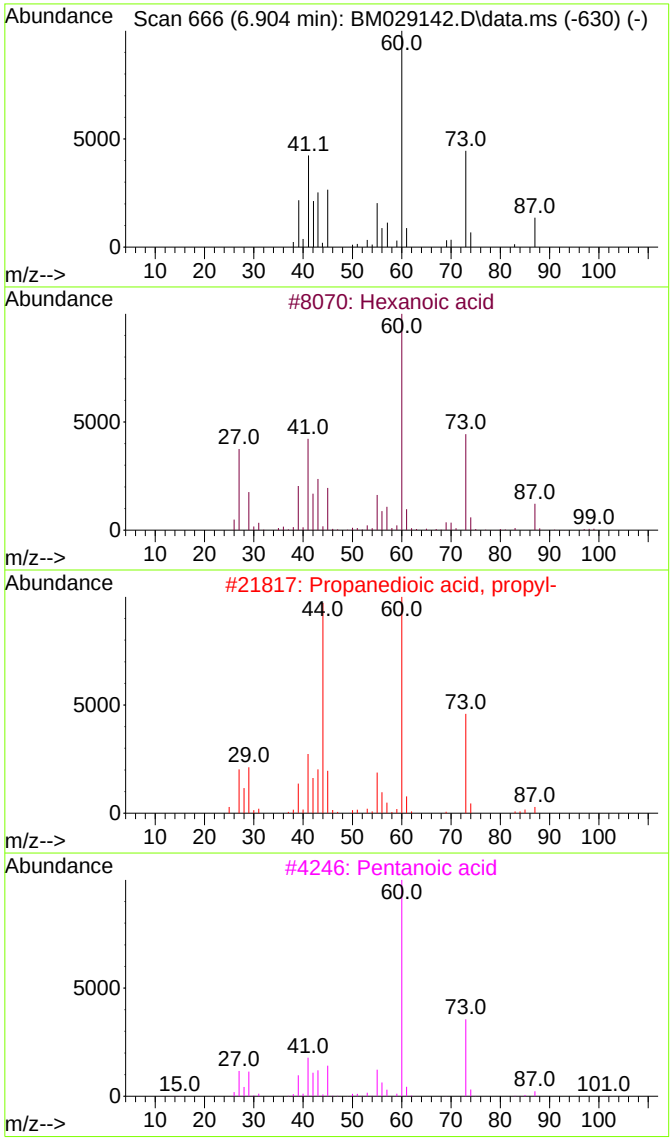
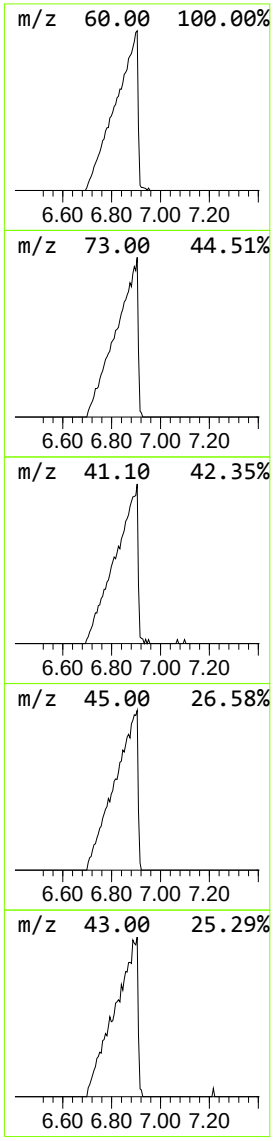
****

Peak Number 3 Hexanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.904	20.00 ng	338770	1,4-Dichlorobenzene-d4	7.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid	116	C6H12O2	000142-62-1	90
2	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	78
3	Pentanoic acid	102	C5H10O2	000109-52-4	50
4	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	42
5	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	23





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Instrument :
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ClientSampleId :
COMP-89-90

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
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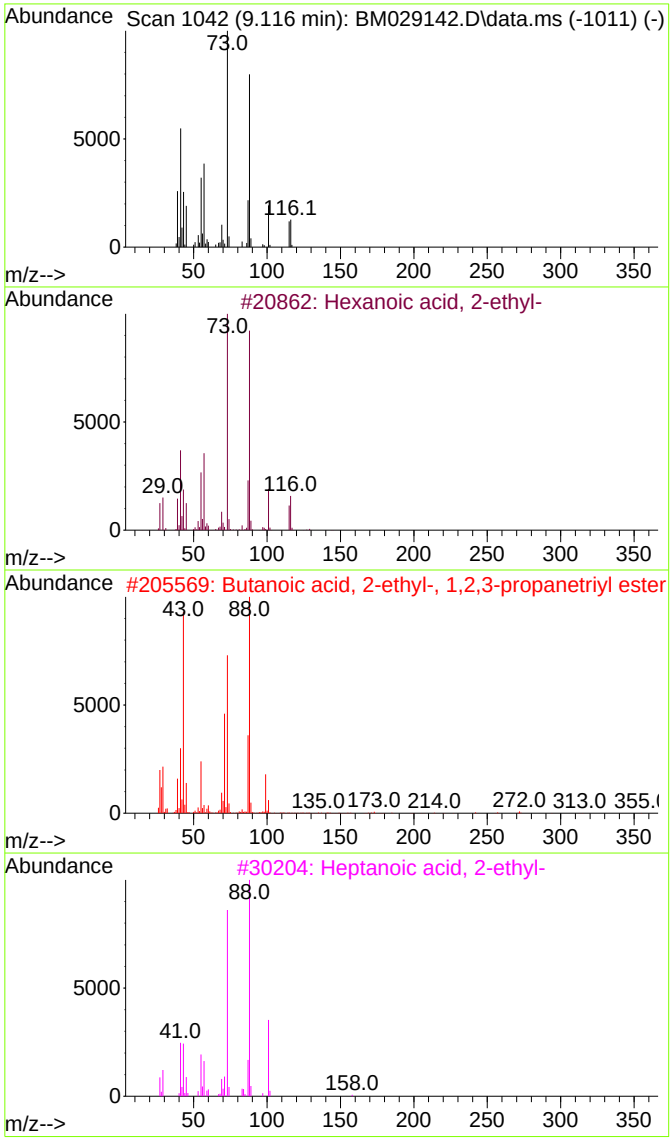
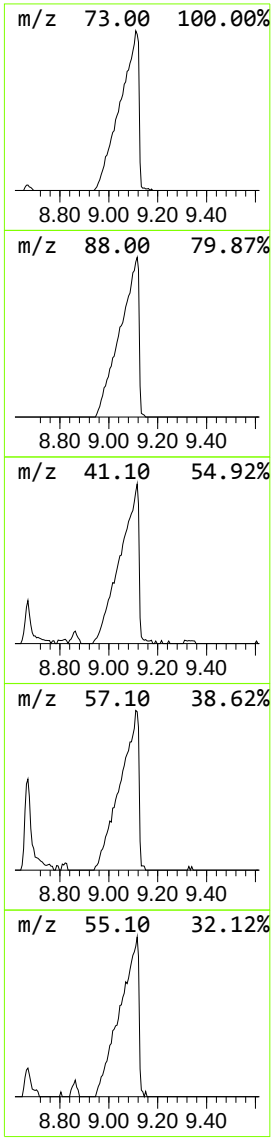
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.116	136.76 ng	469718	Naphthalene-d8	10.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	80
2	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	50
3	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	35
4	1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	32
5	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	25





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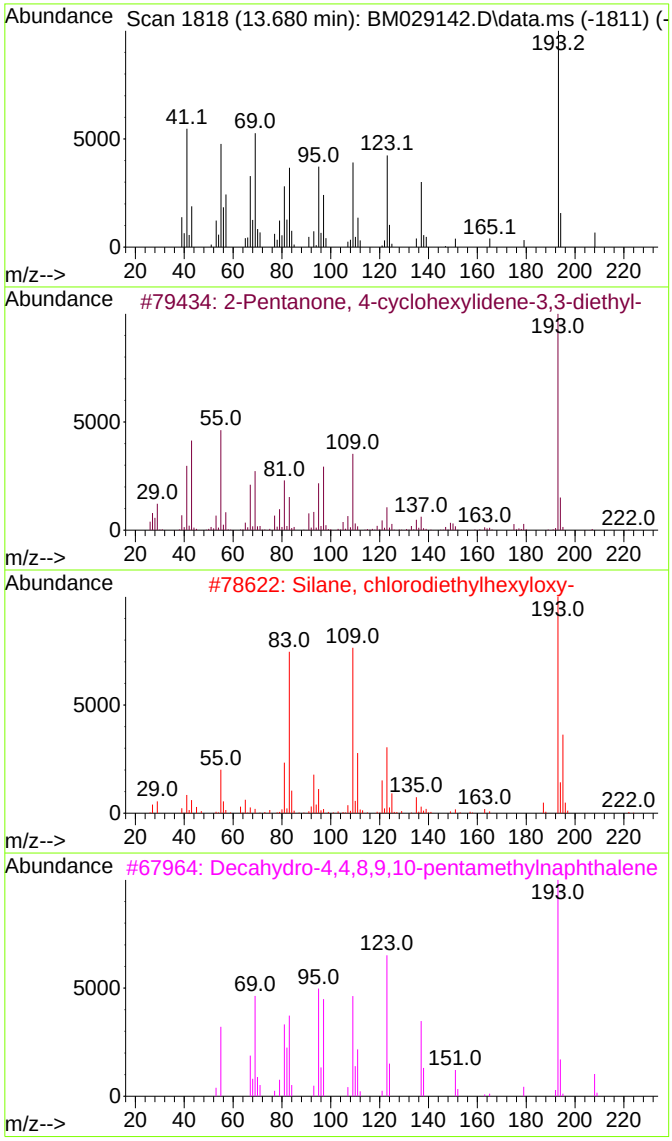
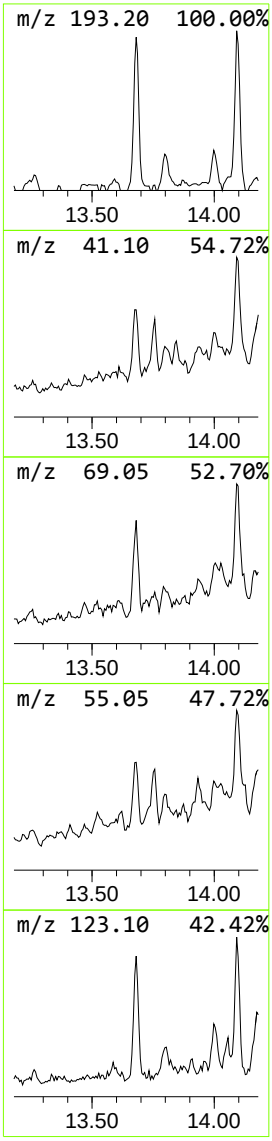
****
Peak Number 5 2-Pentanone, 4-cyclohexylid... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.680	16.94 ng	68818	Acenaphthene-d10	14.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	50
2	Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	35
3	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	30
4	2-Anthracenamine	193	C14H11N	000613-13-8	27
5	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	25





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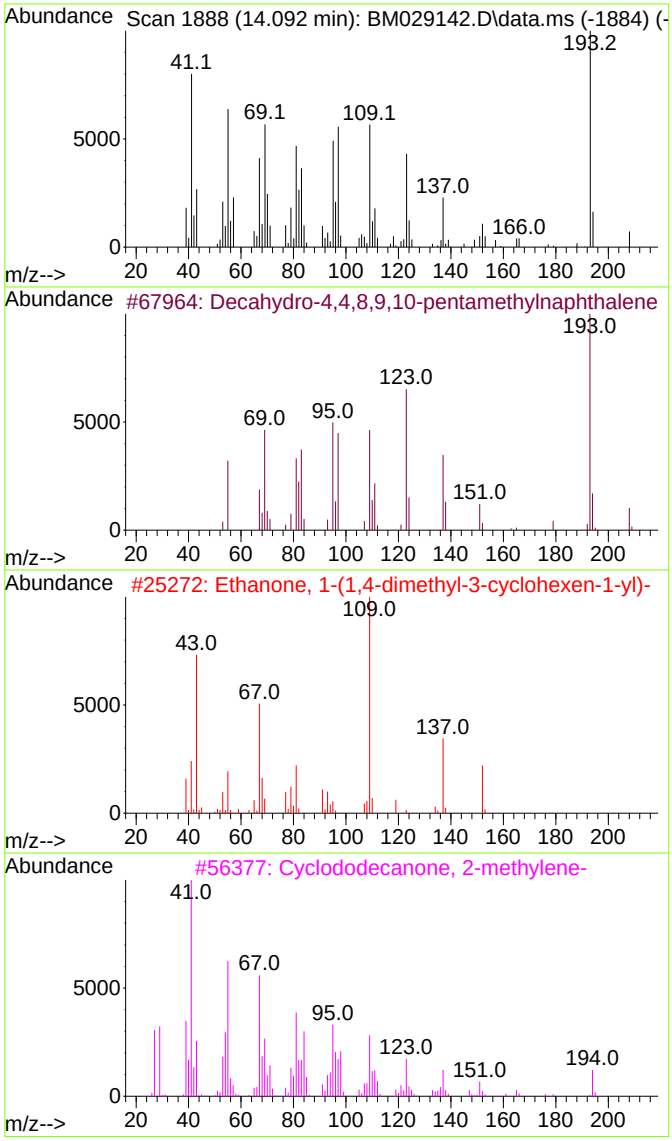
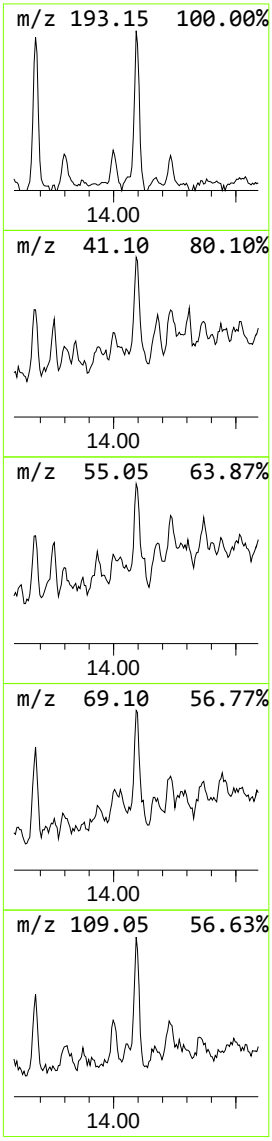
****
Peak Number 6 Decahydro-4,4,8,9,10-pentam... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.092	26.89 ng	109268	Acenaphthene-d10	14.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	60
2	Ethanone, 1-(1,4-dimethyl-3-cycl...	152	C10H16O	043219-68-7	35
3	Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	27
4	2(1H)-Naphthalenone, octahydro-,...	152	C10H16O	016021-08-2	25
5	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	22





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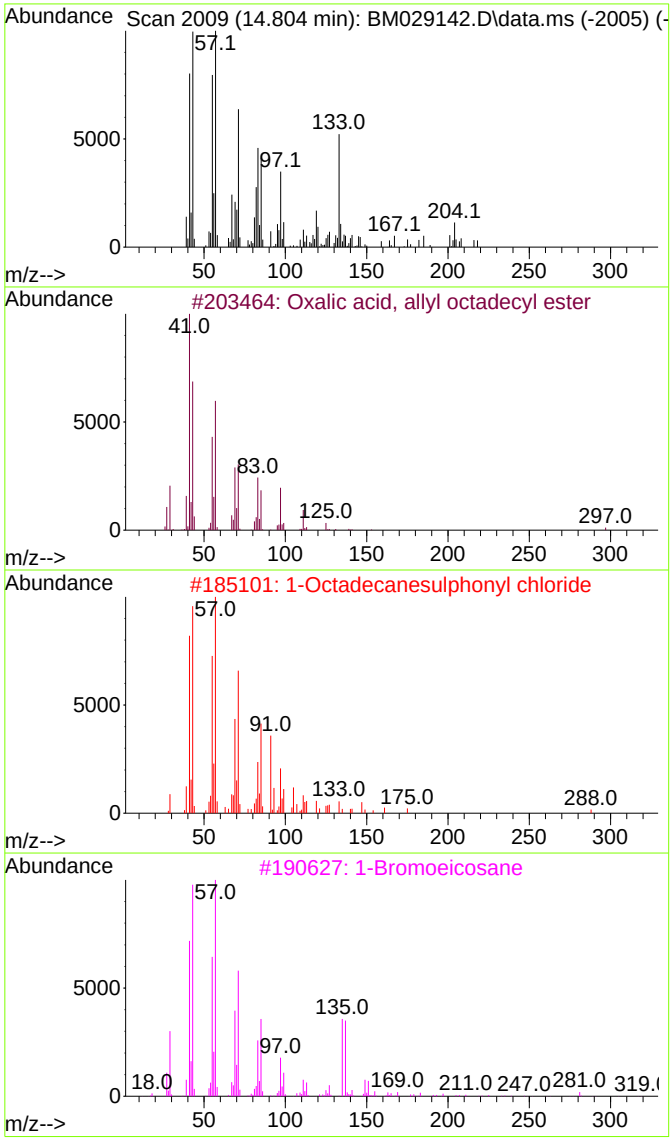
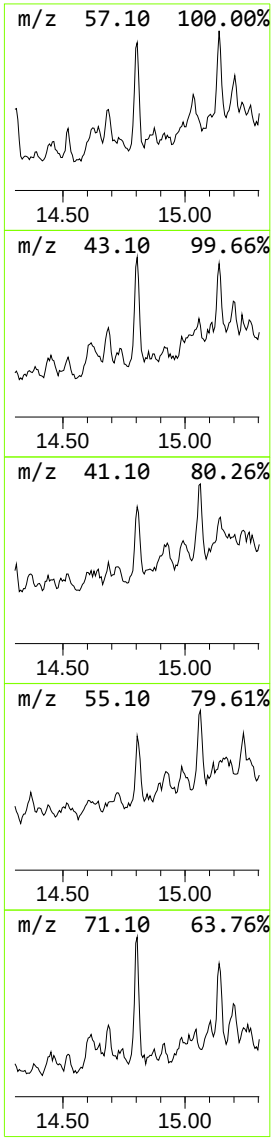
****

Peak Number 7 unknown14.804 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.804	18.99 ng	77157	Acenaphthene-d10	14.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	49
2	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	46
3	1-Bromoeicosane	360	C20H41Br	004276-49-7	41
4	Octadecane, 1-bromo-	332	C18H37Br	000112-89-0	41
5	Pentadecane, 1-bromo-	290	C15H31Br	000629-72-1	41





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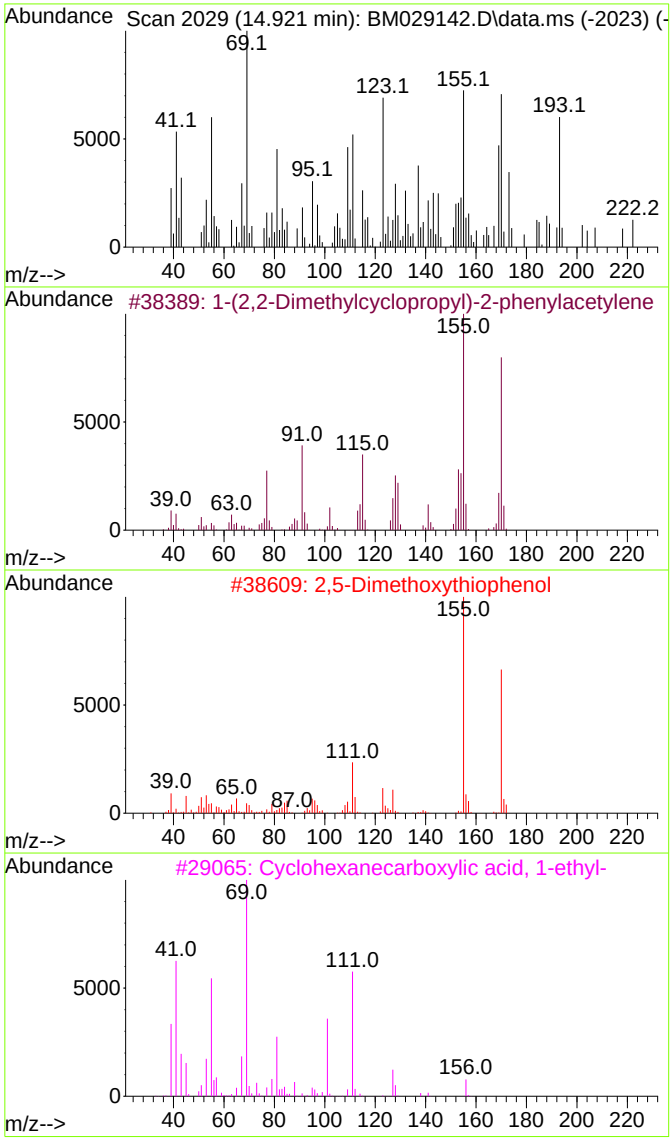
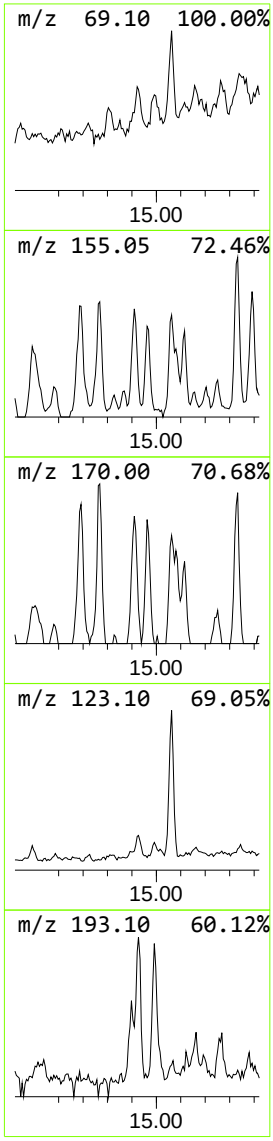
****
Peak Number 8 1-(2,2-Dimethylcyclopropyl)... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.921	20.22 ng	82172	Acenaphthene-d10	14.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(2,2-Dimethylcyclopropyl)-2-ph...	170	C13H14	1000294-91-1	53
2	2,5-Dimethoxythiophenol	170	C8H10O2S	001483-27-8	30
3	Cyclohexanecarboxylic acid, 1-et...	156	C9H16O2	001124-98-7	18
4	Cyclooctane, (1-methylpropyl)-	168	C12H24	016538-89-9	14
5	2,3,4-Trimethyl-hex-3-enal	140	C9H16O	1000193-72-9	14





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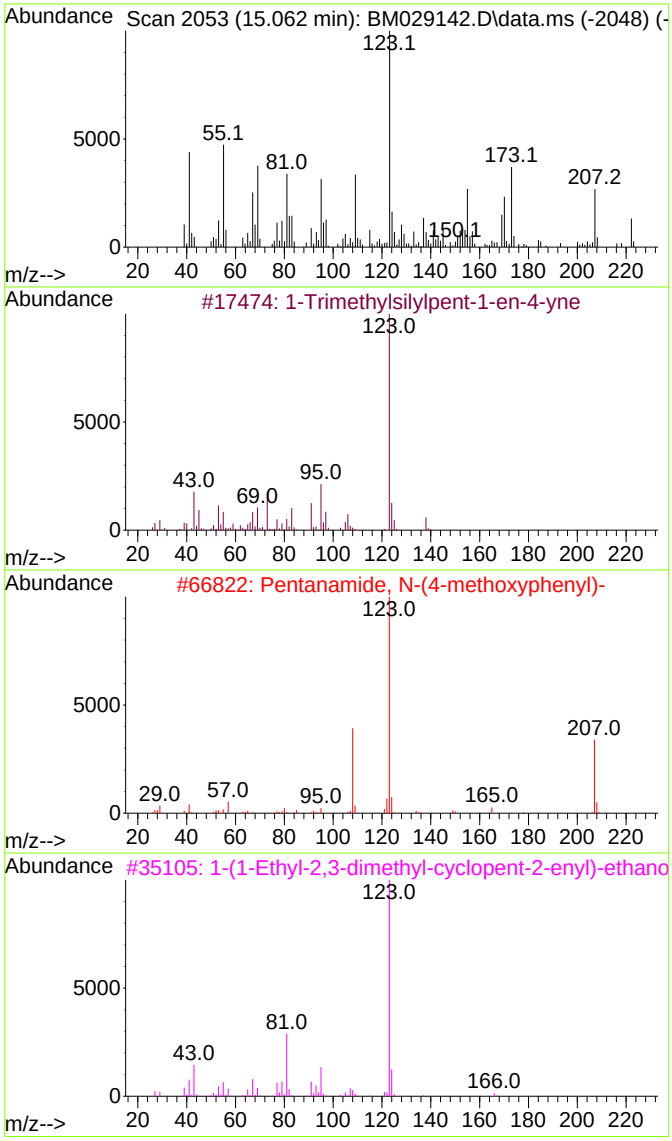
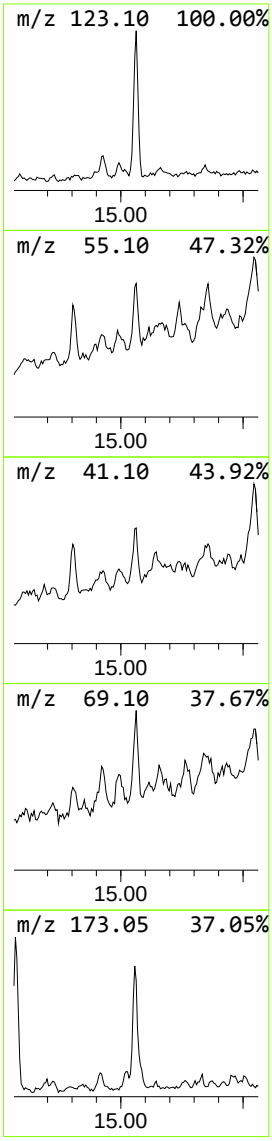
****

Peak Number 9 unknown15.063 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.063	39.08 ng	158815	Acenaphthene-d10	14.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Trimethylsilylpent-1-en-4-yne	138	C8H14Si	079516-25-9	38
2	Pentanamide, N-(4-methoxyphenyl)-	207	C12H17NO2	1000306-89-3	38
3	1-(1-Ethyl-2,3-dimethyl-cyclopen...	166	C11H18O	1000185-18-6	38
4	3-Fluorobenzoic acid, 3-methylbu...	208	C12H13FO2	154559-38-3	38
5	Benzoic acid, 2-fluoro-, ethyl e...	168	C9H9FO2	000443-26-5	35





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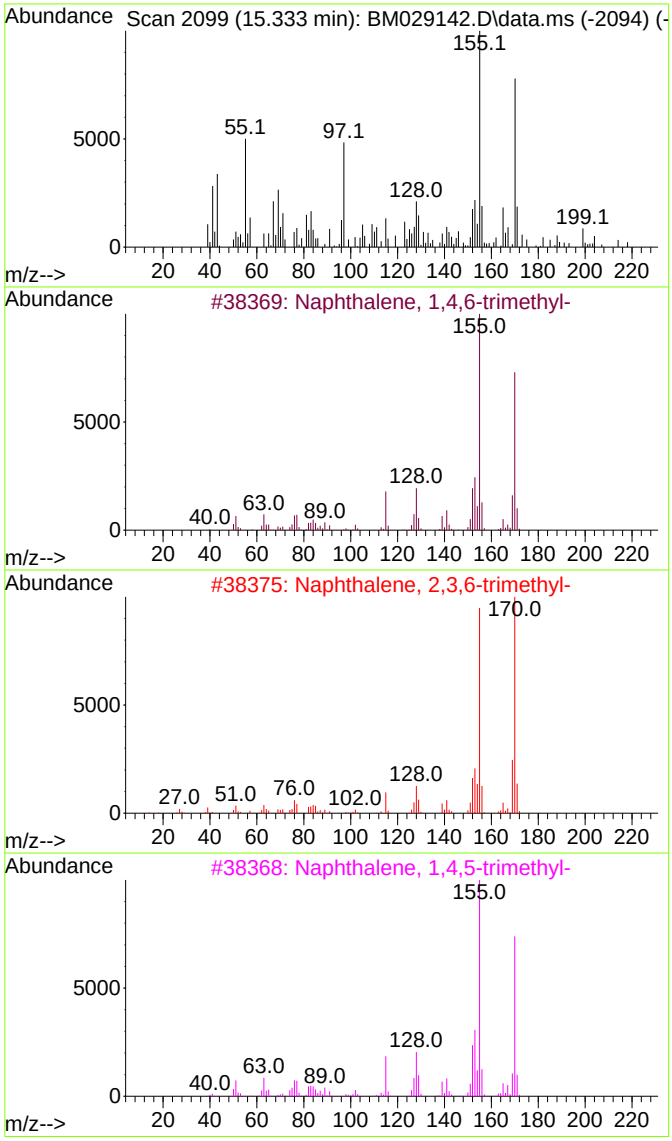
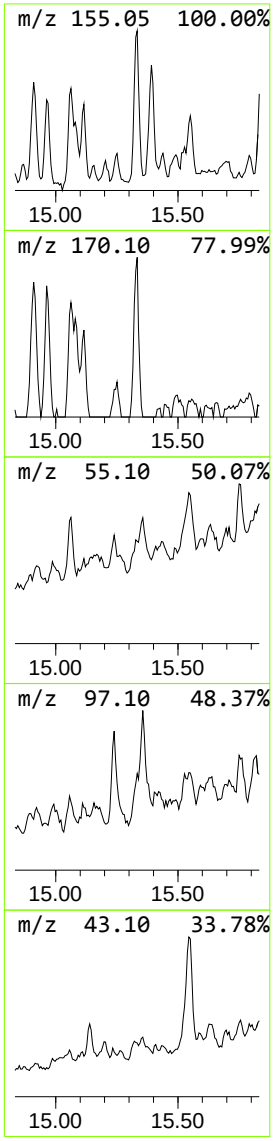
****
Peak Number 10 Naphthalene, 1,4,6-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.333	30.36 ng	123361	Acenaphthene-d10	14.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,4,6-trimethyl-	170	C13H14	002131-42-2	94
2	Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	94
3	Naphthalene, 1,4,5-trimethyl-	170	C13H14	002131-41-1	89
4	Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	76
5	1-(2,2-Dimethylcyclopropyl)-2-ph...	170	C13H14	1000294-91-1	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031521\
Data File : BM029142.D
Acq On : 15 Mar 2021 22:28
Operator : CG/JU
Sample : M1666-05 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-89-90

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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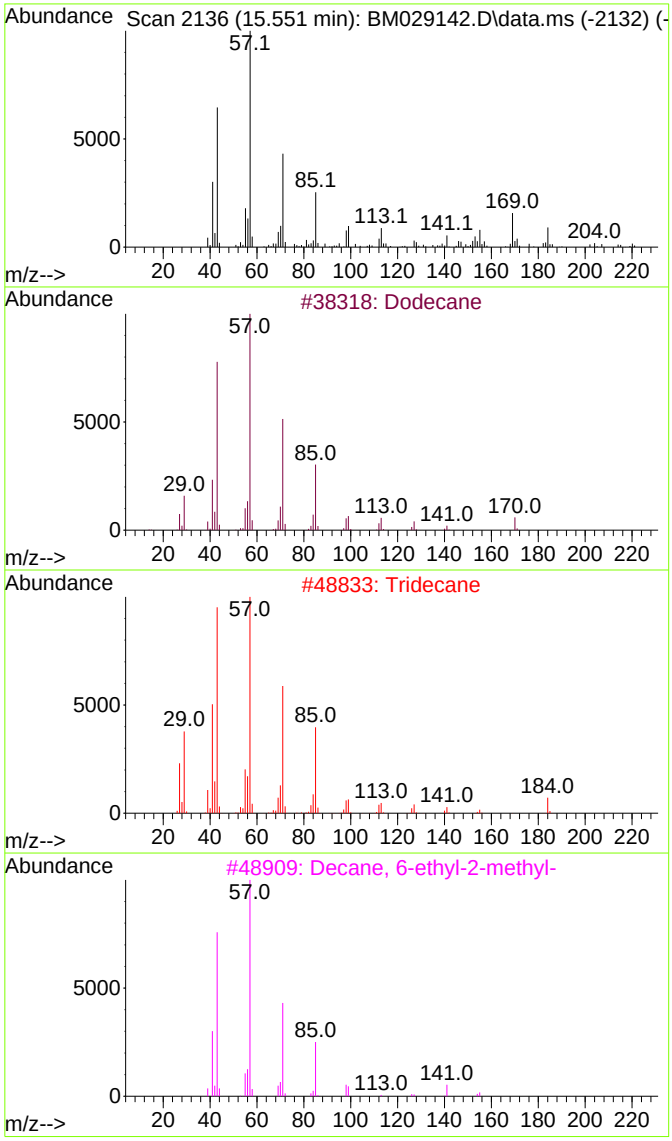
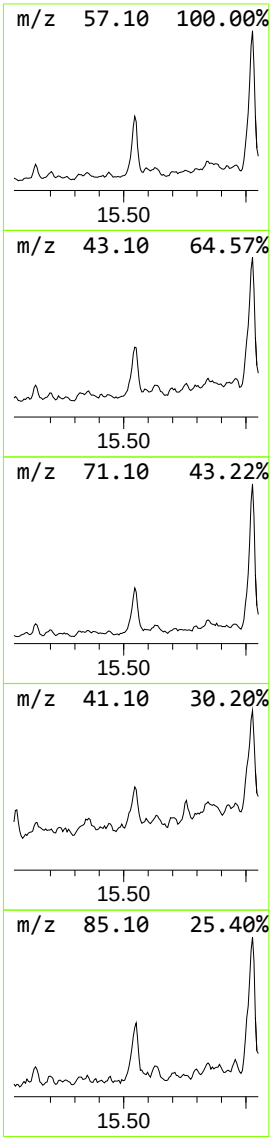
Peak Number 11 Dodecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.551	30.06 ng	122127	Acenaphthene-d10	14.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	70
2	Tridecane	184	C13H28	000629-50-5	62
3	Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	58
4	Undecane	156	C11H24	001120-21-4	58
5	Hexadecane	226	C16H34	000544-76-3	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031521\
Data File : BM029142.D
Acq On : 15 Mar 2021 22:28
Operator : CG/JU
Sample : M1666-05 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-89-90

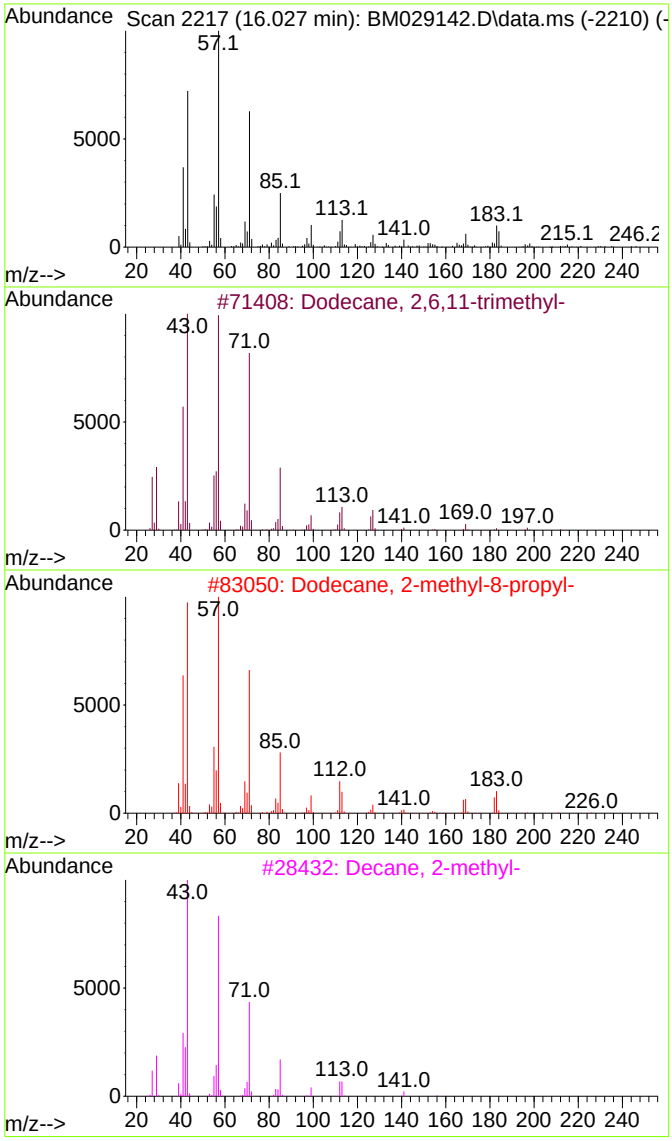
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

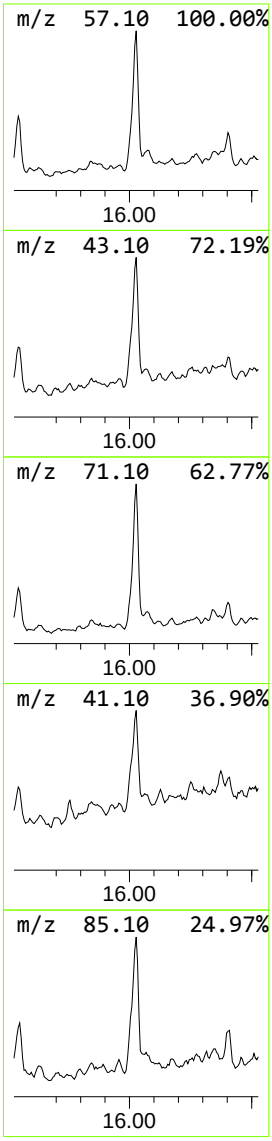
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Dodecane, 2,6,11-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.027	49.55 ng	455134	Phenanthrene-d10	17.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	86
2	Dodecane, 2-methyl-8-propyl-	226	C16H34	055045-07-3	86
3	Decane, 2-methyl-	156	C11H24	006975-98-0	76
4	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	72
5	3,5-Heptanedione, 2,2,4,6-tetram...	184	C11H20O2	1000162-24-5	68





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Data File : BM029142.D
Acq On : 15 Mar 2021 22:28
Operator : CG/JU
Sample : M1666-05 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : COMP-89-90

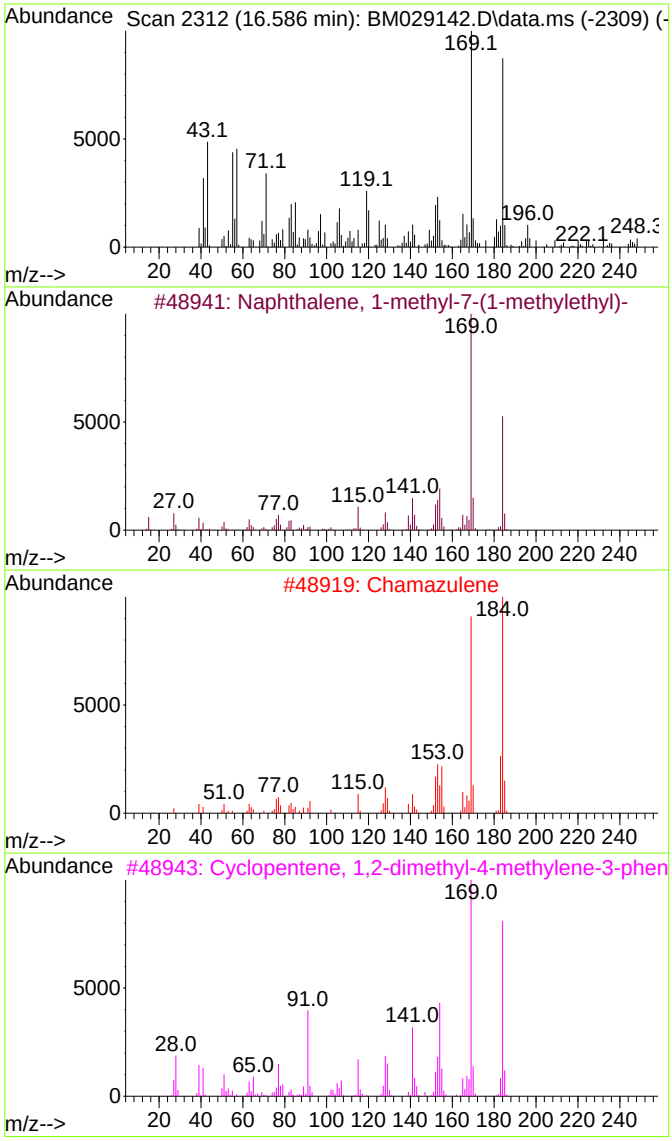
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

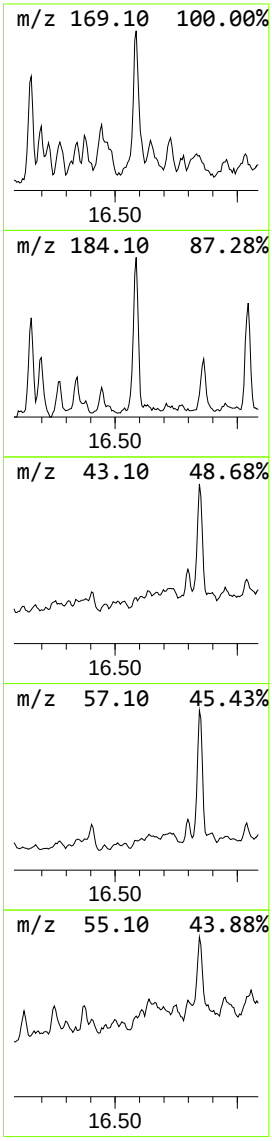
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Naphthalene, 1-methyl-7-(1-... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.586	8.18 ng	75144	Phenanthrene-d10	17.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-7-(1-methy...	184	C14H16	000490-65-3	93
2	Chamazulene	184	C14H16	000529-05-5	93
3	Cyclopentene, 1,2-dimethyl-4-met...	184	C14H16	1000152-22-4	76
4	Naphthalene, 1,2,3,4-tetramethyl-	184	C14H16	003031-15-0	58
5	1,4,5,8-Tetramethylnaphthalene	184	C14H16	002717-39-7	50





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Data File : BM029142.D
Acq On : 15 Mar 2021 22:28
Operator : CG/JU
Sample : M1666-05 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-89-90

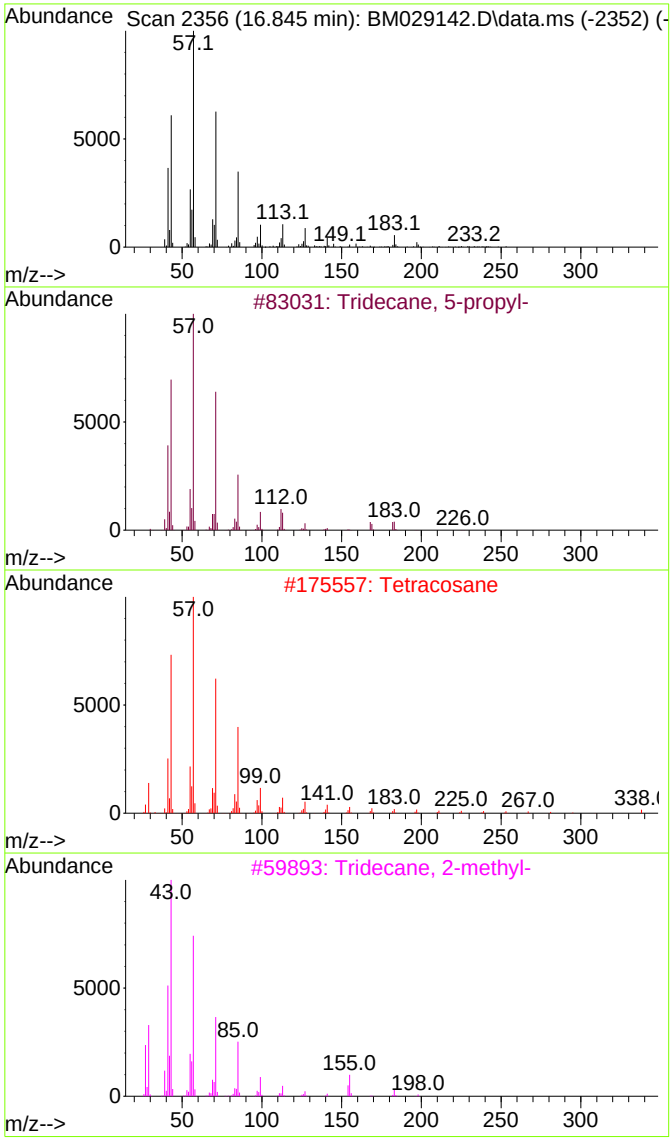
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

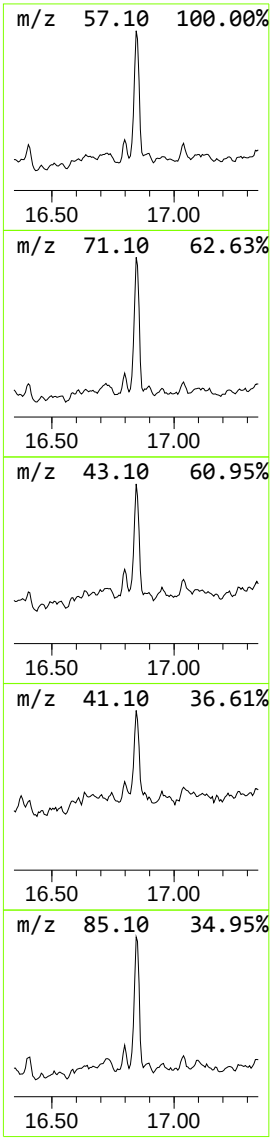
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Tridecane, 5-propyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.845	50.32 ng	462200	Phenanthrene-d10	17.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 5-propyl-	226	C16H34	055045-11-9	90
2	Tetracosane	338	C24H50	000646-31-1	86
3	Tridecane, 2-methyl-	198	C14H30	001560-96-9	86
4	Tridecane, 6-propyl-	226	C16H34	055045-10-8	81
5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031521\
Data File : BM029142.D
Acq On : 15 Mar 2021 22:28
Operator : CG/JU
Sample : M1666-05 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : COMP-89-90

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.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
unknown3.857	3.857	7.0	ng	118935	1	7.616	338770	20.0
Ethanol, 2-butoxy-	5.763	335.1	ng	5676910	1	7.616	338770	20.0
Hexanoic acid	6.904	20.0	ng	338770	1	7.616	338770	20.0
Hexanoic acid, ...	9.116	136.8	ng	469718	2	10.404	68691	20.0
2-Pentanone, 4-...	13.680	16.9	ng	68818	3	14.286	81269	20.0
Decahydro-4,4,8...	14.092	26.9	ng	109268	3	14.286	81269	20.0
unknown14.804	14.804	19.0	ng	77157	3	14.286	81269	20.0
1-(2,2-Dimethyl...	14.921	20.2	ng	82172	3	14.286	81269	20.0
unknown15.063	15.063	39.1	ng	158815	3	14.286	81269	20.0
Naphthalene, 1,...	15.333	30.4	ng	123361	3	14.286	81269	20.0
Dodecane	15.551	30.1	ng	122127	3	14.286	81269	20.0
Dodecane, 2,6,1...	16.027	49.5	ng	455134	4	17.045	183699	20.0
Naphthalene, 1-...	16.586	8.2	ng	75144	4	17.045	183699	20.0
Tridecane, 5-pr...	16.845	50.3	ng	462200	4	17.045	183699	20.0