LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
Data File : BM018929.D
Acq On : 26 Feb 2019 14:56
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-022019

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-BM021119.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	7.234	699	705	710	rBV	870298	1267789	1.05%	0.472%
2	7.475	740	746	770	rVB	995959	1730748	1.44%	0.644%
3	7.692	776	783	792	rBV	920740	1471225	1.22%	0.548%
4	9.851	1145	1150	1154	rBV	841494	1351615	1.12%	0.503%
5	10.081	1184	1189	1193	rBV	770812	1357951	1.13%	0.506%
6	10.175	1199	1205	1206	rBV3	1340436	2095044	1.74%	0.780%
7	10.292	1220	1225	1227	rBV2	1550619	2513563	2.09%	0.936%
8	10.322	1227	1230	1235	rVV2	2352874	5057676	4.20%	1.883%
9	10.369	1235	1238	1246	rVV5	1471456	3395142	2.82%	1.264%
10	10.457	1246	1253	1267	rVB2	2919993	8195212	6.81%	3.051%
11	10.645	1281	1285	1287	rVV	1298505	1974041	1.64%	0.735%
12	10.681	1287	1291	1300	rVB2	2112813	4052850	3.37%	1.509%
13	10.863	1310	1322	1329	rBV4	1452567	4779537	3.97%	1.780%
14	11.504	1424	1431	1451	rVB	4402257	7162824	5.95%	2.667%
15	14.016	1846	1858	1862	rBV	54487215	120284719	100.00%	44.787%
16	14.345	1908	1914	1923	rVB2	1502625	2400837	2.00%	0.894%
17	15.898	2170	2178	2200	rBV	41061891	58898142	48.97%	21.930%
18	17.098	2372	2382	2391	rBV	1832469	2530091	2.10%	0.942%
19	17.468	2440	2445	2460	rBV	9305274	13813648	11.48%	5.143%
20	18.721	2654	2658	2661	rBV2	916006	1230316	1.02%	0.458%
21	18.845	2674	2679	2695	rVB2	1369311	2727512	2.27%	1.016%
22	19.733	2825	2830	2841	rBV4	716438	1304435	1.08%	0.486%
23	20.133	2893	2898	2906	rBV	1273378	1490538	1.24%	0.555%
24	21.033	3047	3051	3060	rBV	1610067	2471508	2.05%	0.920%
25	21.127	3063	3067	3073	rVB	1137076	1283201	1.07%	0.478%
26	21.292	3089	3095	3105	rBV2	2433830	3752317	3.12%	1.397%
27	21.415	3112	3116	3127	rBV	888860	1906428	1.58%	0.710%
28	22.721	3334	3338	3351	rVB	1164928	2161023	1.80%	0.805%
29	22.827	3352	3356	3363	rVB	1079495	1607919	1.34%	0.599%
30	23.539	3472	3477	3487	rVB	1569768	3032198	2.52%	1.129%
31	24.044	3558	3563	3571	rVB	675499	1272538	1.06%	0.474%

Sum of corrected areas: 268572587

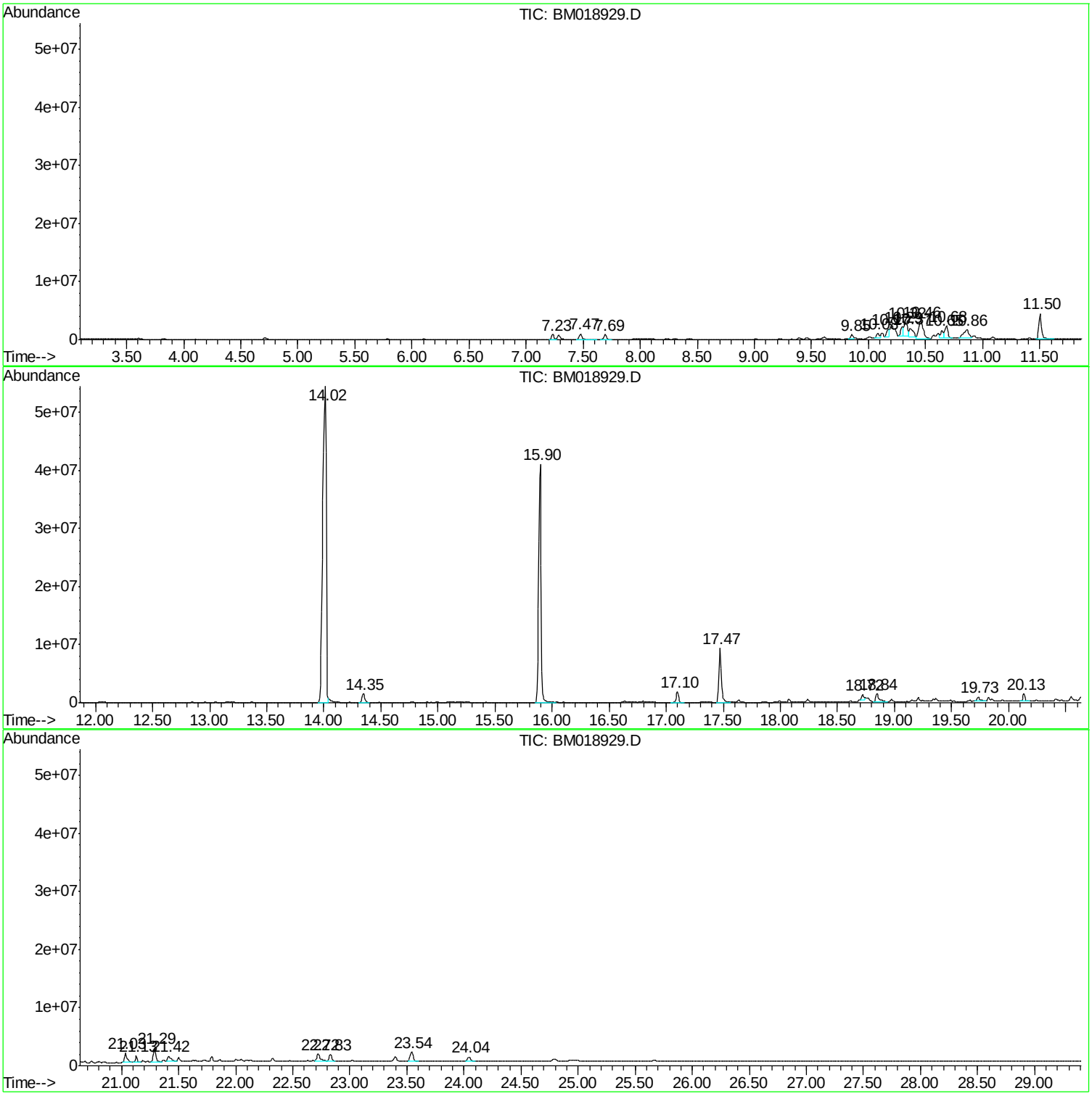
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
Data File : BM018929.D
Acq On : 26 Feb 2019 14:56
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
Data File : BM018929.D
Acq On : 26 Feb 2019 14:56
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

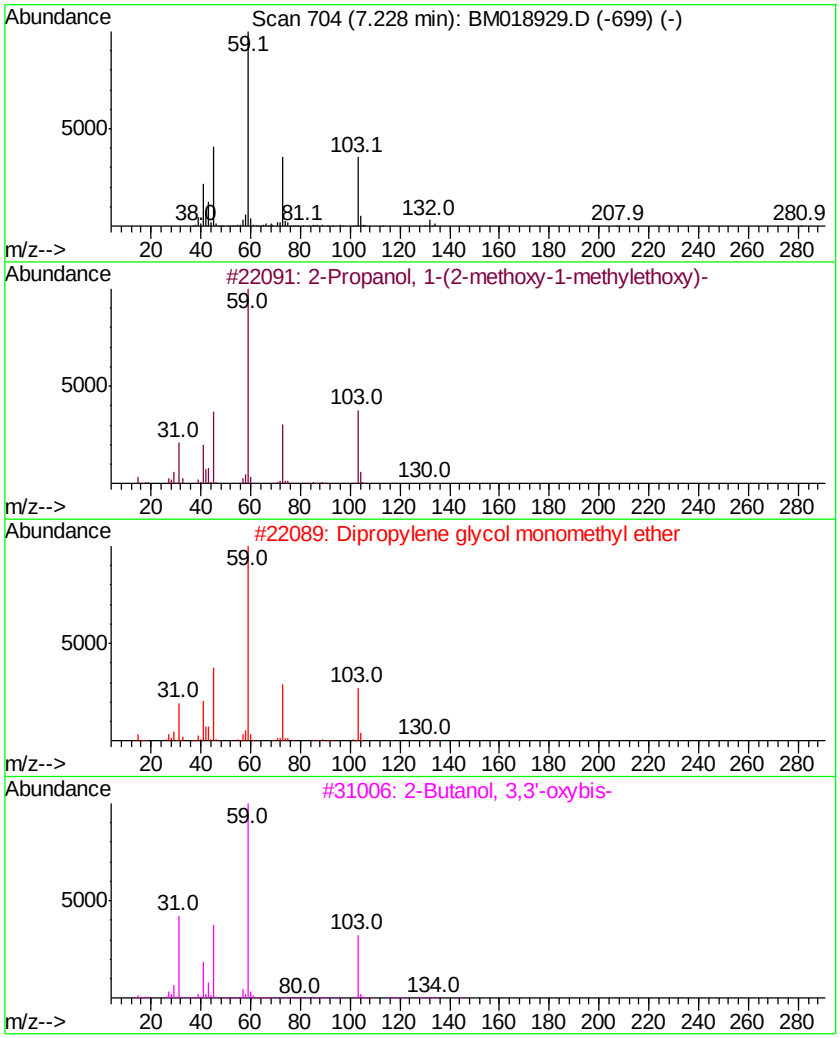
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

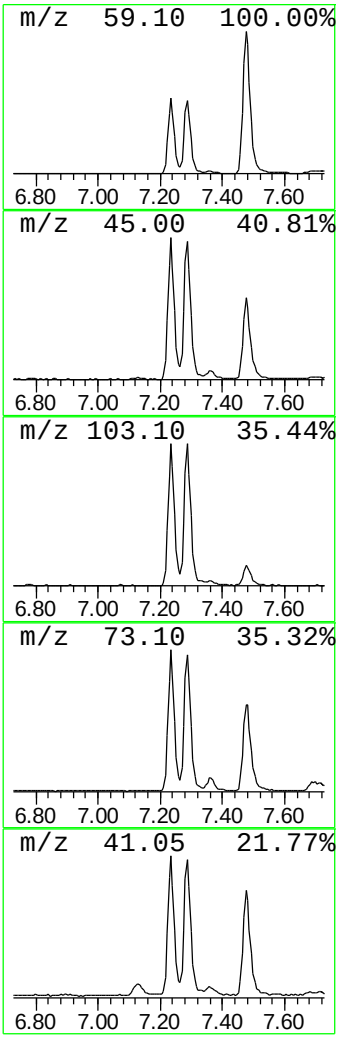
****

Peak Number 1 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.23	17.23 ng	1267790	1,4-Dichlorobenzene-d4	7.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	90
2	Dipropylene glycol monomethyl ether	148	C7H16O3	034590-94-8	83
3	2-Butanol, 3,3'-oxybis-	162	C8H18O3	054305-61-2	64
4	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	53
5	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	50





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
Data File : BM018929.D
Acq On : 26 Feb 2019 14:56
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

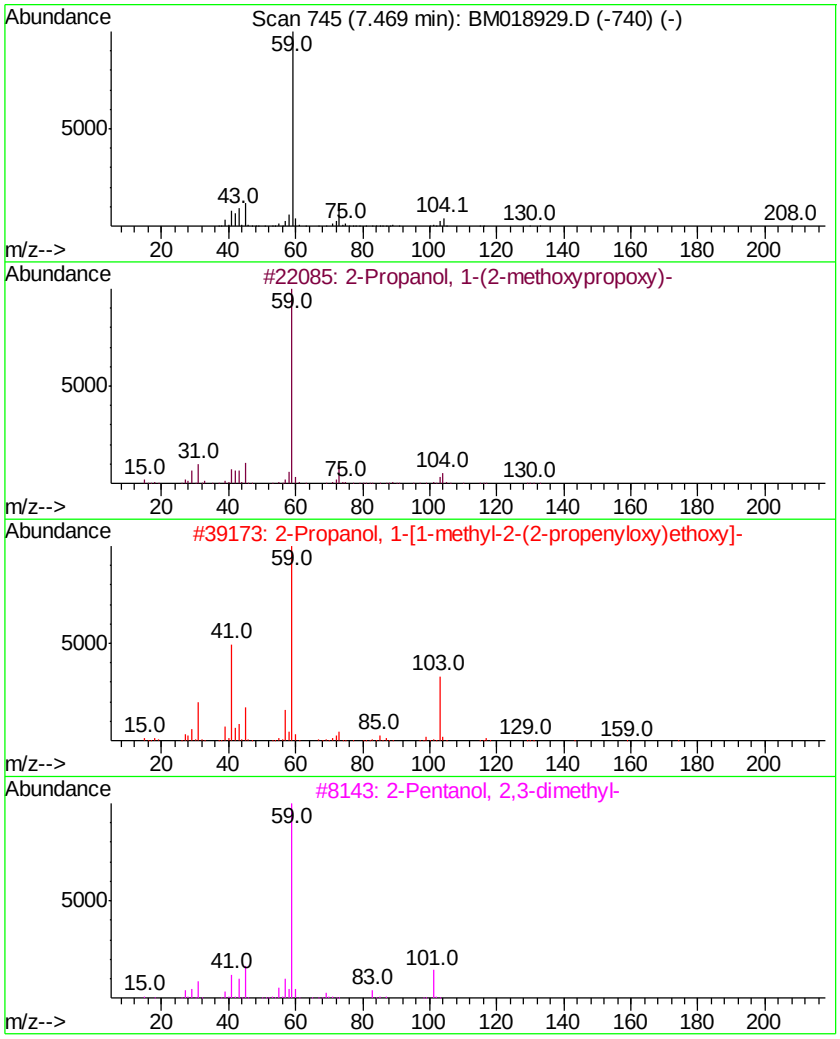
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

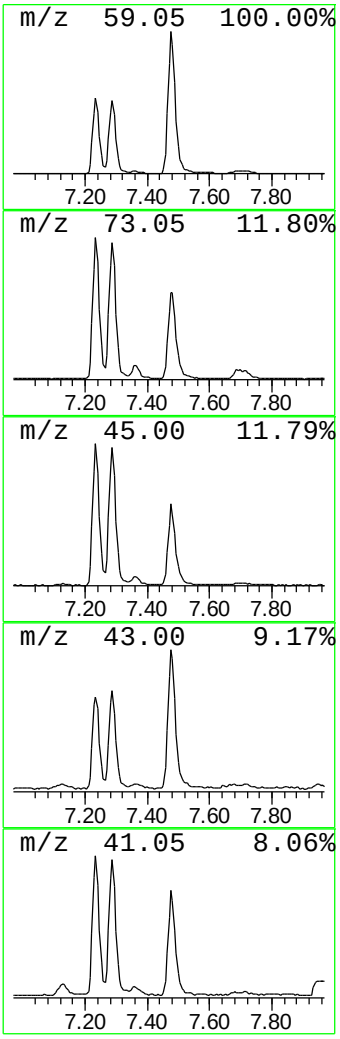
****

Peak Number 2 2-Propanol, 1-(2-methoxypro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.47	23.53 ng	1730750	1,4-Dichlorobenzene-d4	7.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	83
2	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	78
3	2-Pentanol, 2,3-dimethyl-	116	C7H16O	004911-70-0	50
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	40
5	3-Hexanol	102	C6H14O	000623-37-0	40





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
Data File : BM018929.D
Acq On : 26 Feb 2019 14:56
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

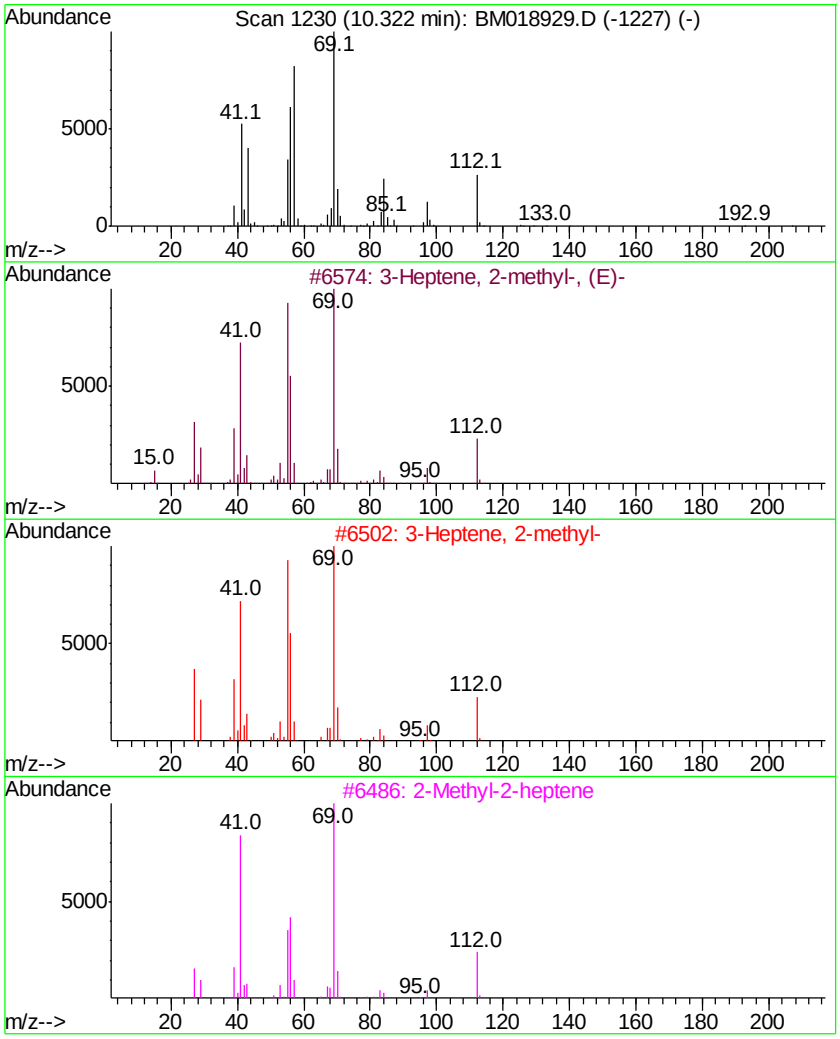
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

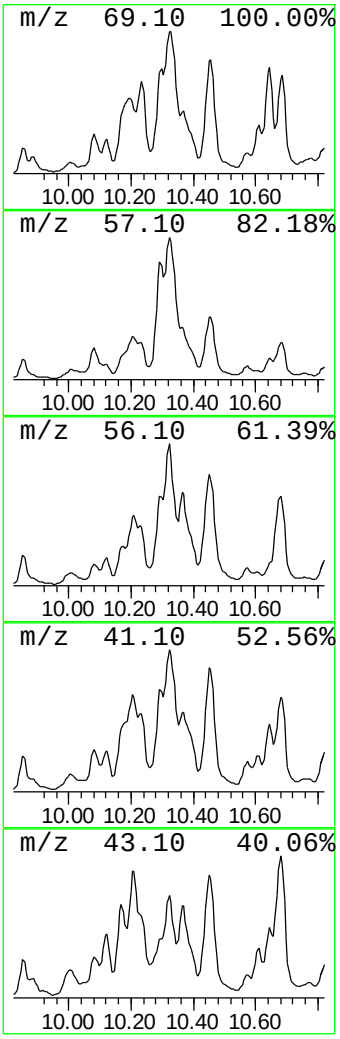
****

Peak Number 3 3-Heptene, 2-methyl-, (E)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.32	12.34 ng	5057680	Naphthalene-d8	10.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptene, 2-methyl-, (E)-	112	C8H16	000692-96-6	72
2	3-Heptene, 2-methyl-	112	C8H16	017618-76-7	68
3	2-Methyl-2-heptene	112	C8H16	000627-97-4	50
4	Cyclohexanone, 3-methyl-, (R)-	112	C7H12O	013368-65-5	50
5	Ornithine	132	C5H12N2O2	000070-26-8	50





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
Data File : BM018929.D
Acq On : 26 Feb 2019 14:56
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

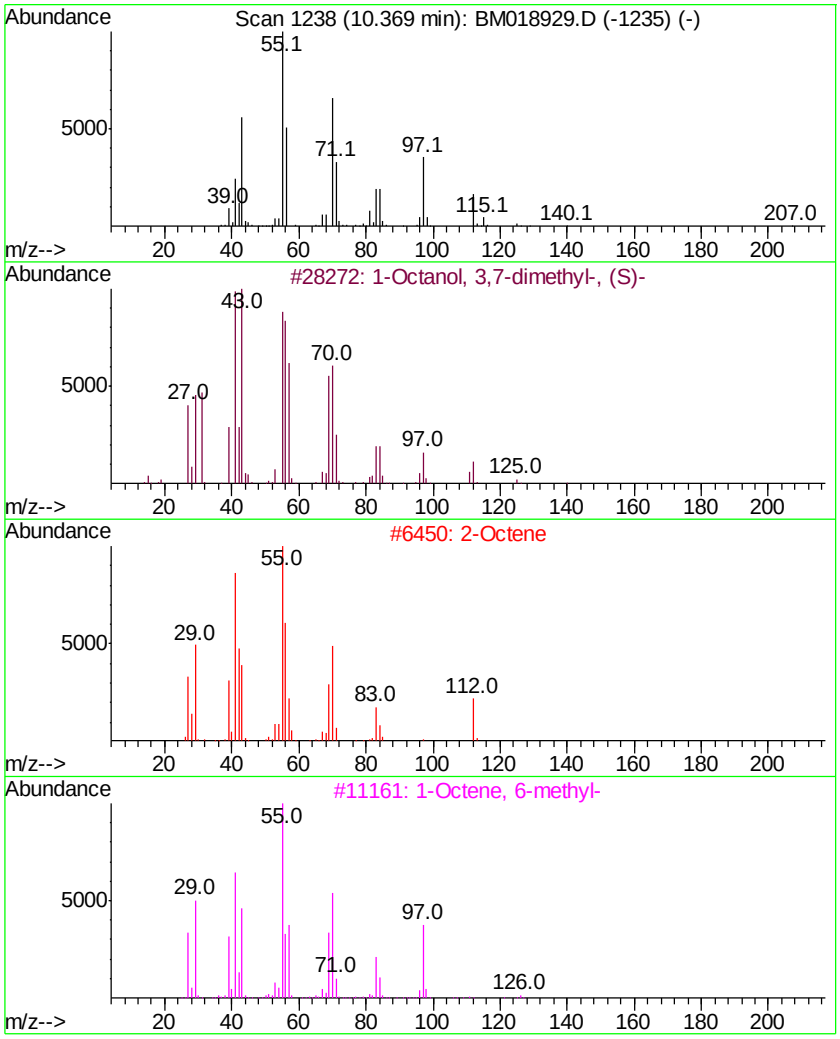
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

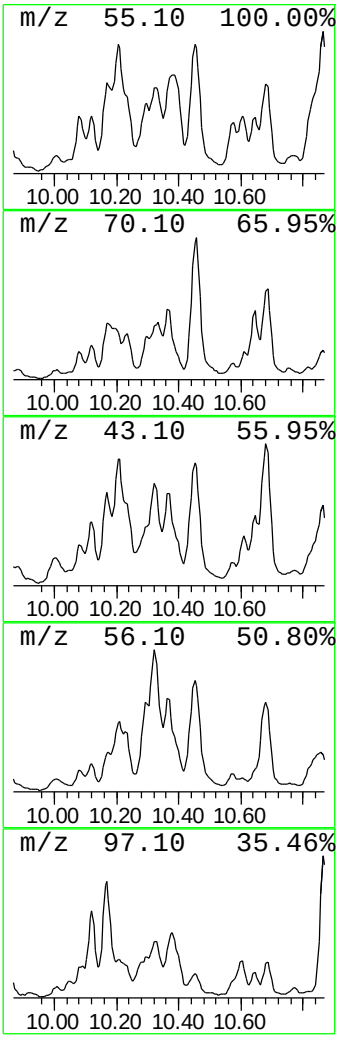
****

Peak Number 4 1-Octanol, 3,7-dimethyl-, (S)- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.37	8.29 ng	3395140	Naphthalene-d8	10.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol, 3,7-dimethyl-, (S)-	158	C10H22O	068680-98-8	78
2	2-Octene	112	C8H16	000111-67-1	64
3	1-Octene, 6-methyl-	126	C9H18	013151-10-5	59
4	1-Octene	112	C8H16	000111-66-0	50
5	Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	015890-40-1	50





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
Data File : BM018929.D
Acq On : 26 Feb 2019 14:56
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

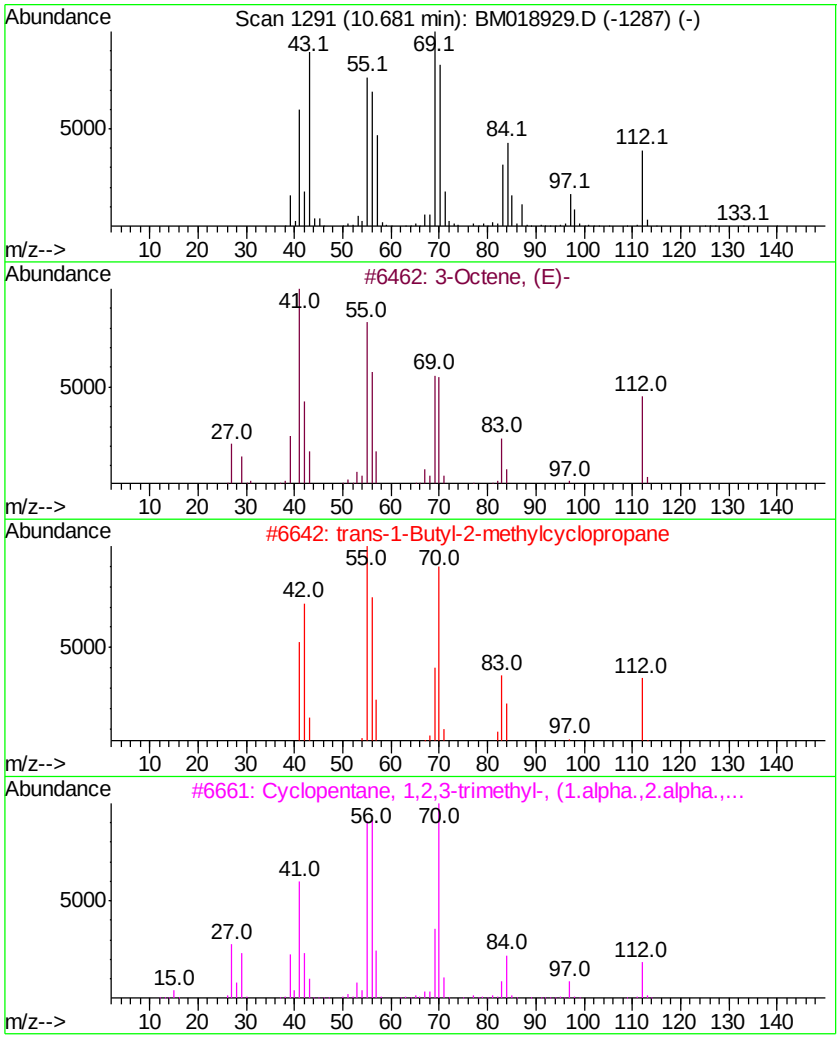
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

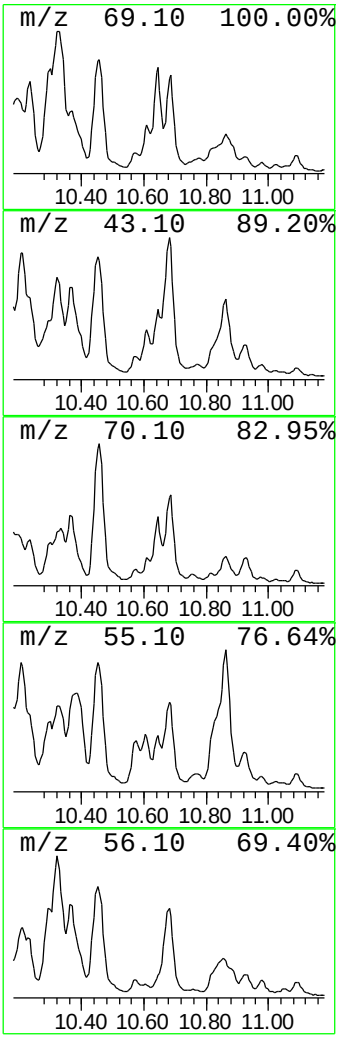
****

Peak Number 5 3-Octene, (E)- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.68	9.89 ng	4052850	Naphthalene-d8	10.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octene, (E)-	112	C8H16	014919-01-8	74
2	trans-1-Butyl-2-methylcyclopropane	112	C8H16	038851-70-6	53
3	Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	015890-40-1	50
4	2-Octene, (Z)-	112	C8H16	007642-04-8	49
5	1-Heptene, 6-methyl-	112	C8H16	005026-76-6	49





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
Data File : BM018929.D
Acq On : 26 Feb 2019 14:56
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

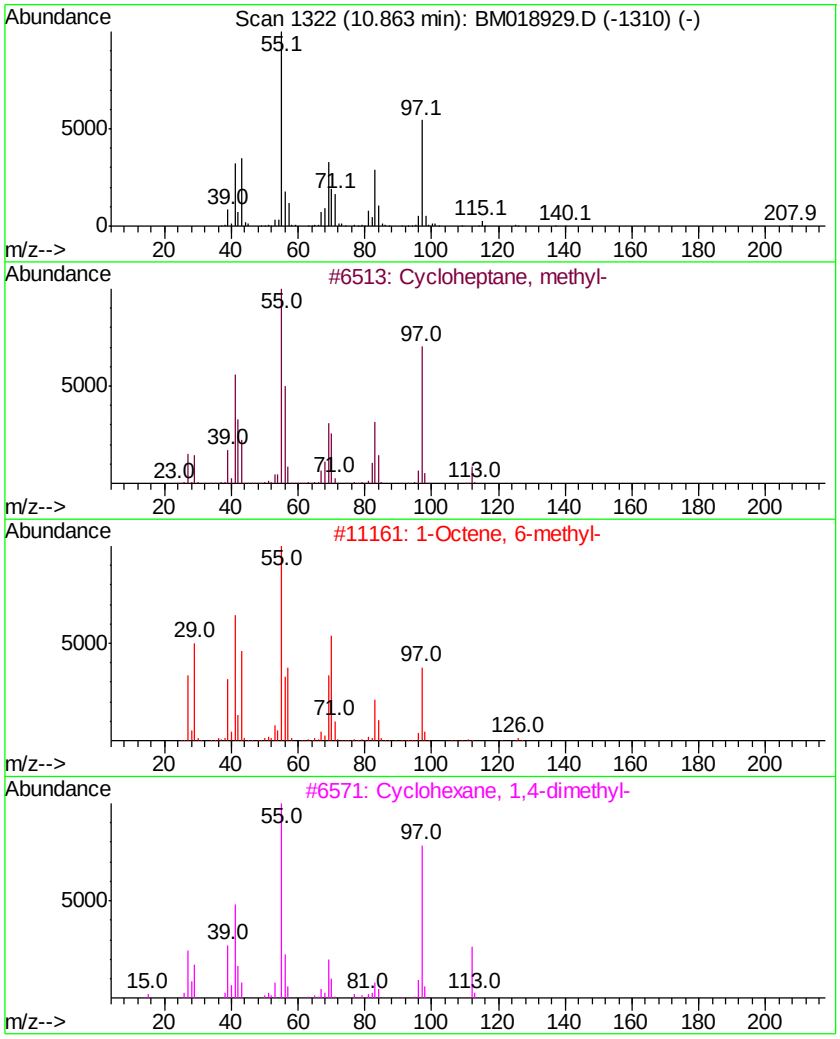
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

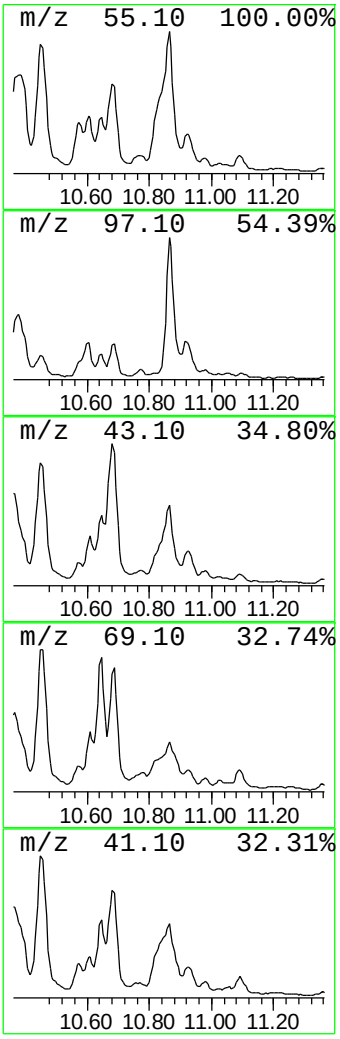
****

Peak Number 6 Cycloheptane, methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.86	11.66 ng	4779540	Naphthalene-d8	10.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloheptane, methyl-	112	C8H16	004126-78-7	56
2	1-Octene, 6-methyl-	126	C9H18	013151-10-5	53
3	Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	50
4	Cyclohexane, 1,2-dimethyl-	112	C8H16	000583-57-3	50
5	Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	47





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
Data File : BM018929.D
Acq On : 26 Feb 2019 14:56
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

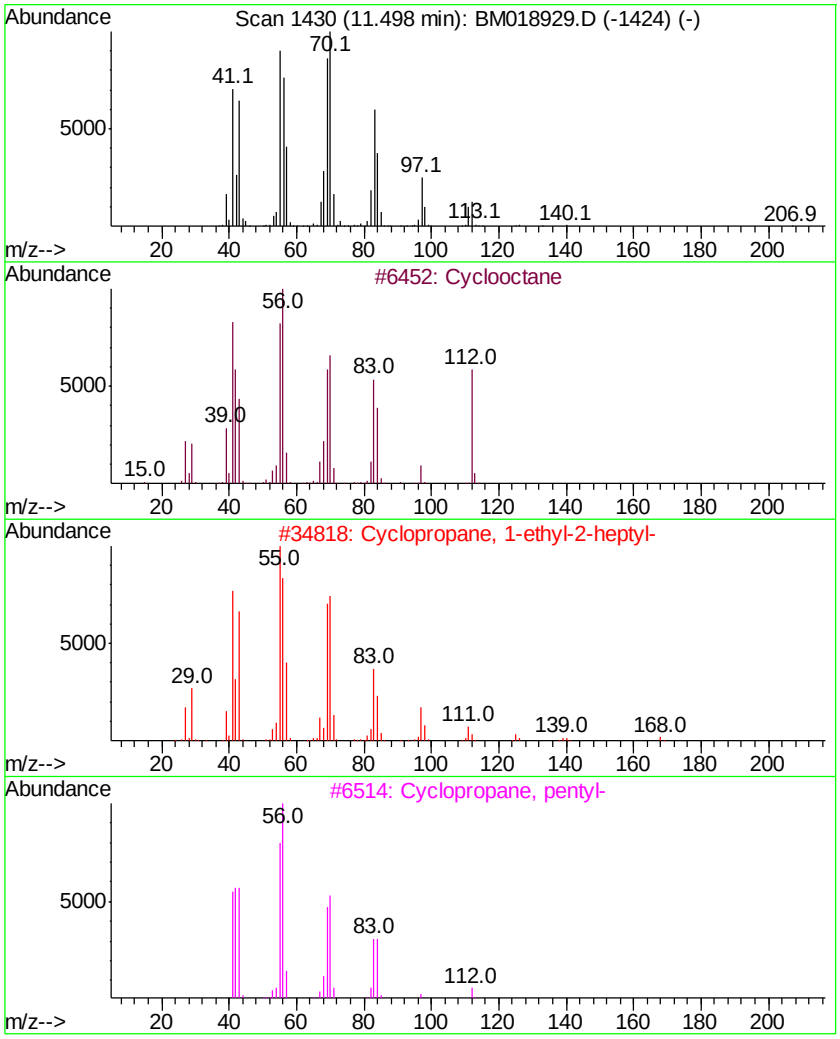
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

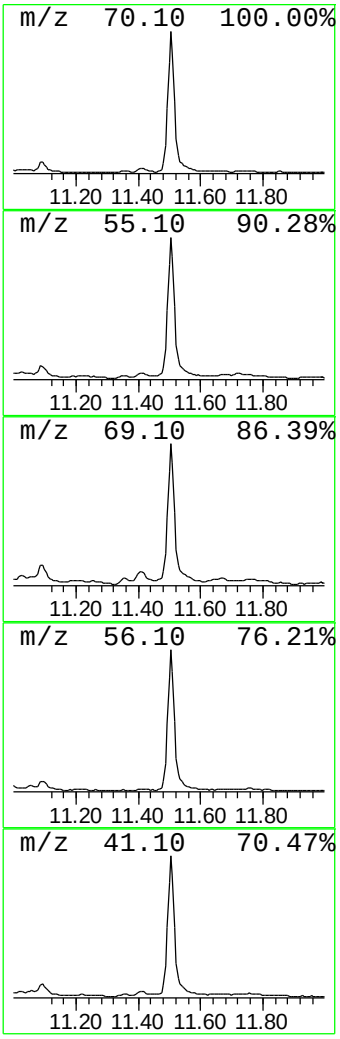
****

Peak Number 7 Cyclooctane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.50	17.48 ng	7162820	Naphthalene-d8	10.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclooctane	112	C8H16	000292-64-8	60
2	Cyclopropane, 1-ethyl-2-heptyl-	168	C12H24	074663-86-8	50
3	Cyclopropane, pentyl-	112	C8H16	002511-91-3	49
4	Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	015890-40-1	43
5	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	43





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
Data File : BM018929.D
Acq On : 26 Feb 2019 14:56
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

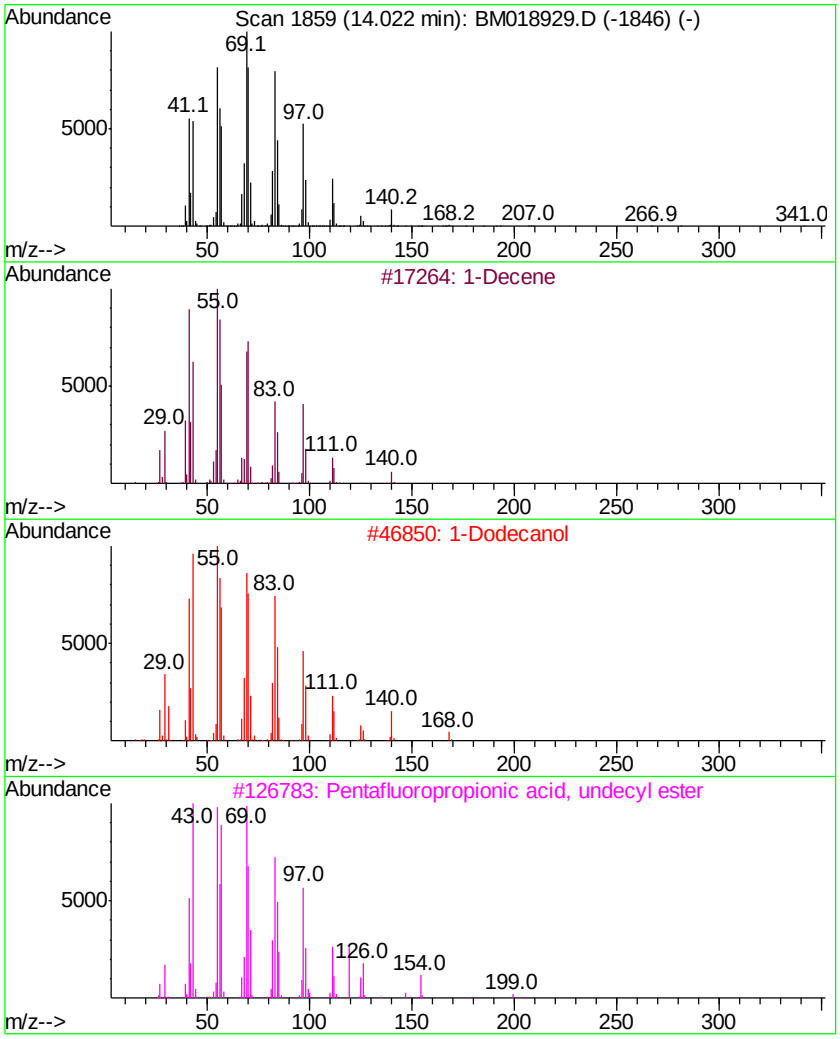
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

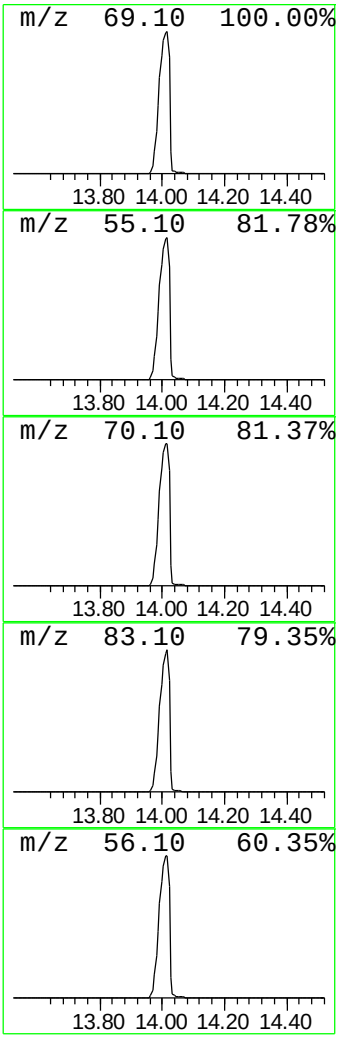
****

Peak Number 8 1-Decene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.02	1002.02 ng	120285000	Acenaphthene-d10	14.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decene	140	C10H20	000872-05-9	94
2	1-Dodecanol	186	C12H26O	000112-53-8	91
3	Pentafluoropropionic acid, undec...	318	C14H23F5O2	1000283-04-0	90
4	1-Tridecanol	200	C13H28O	000112-70-9	90
5	Cyclodecane, methyl-	154	C11H22	013151-43-4	89





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
Data File : BM018929.D
Acq On : 26 Feb 2019 14:56
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

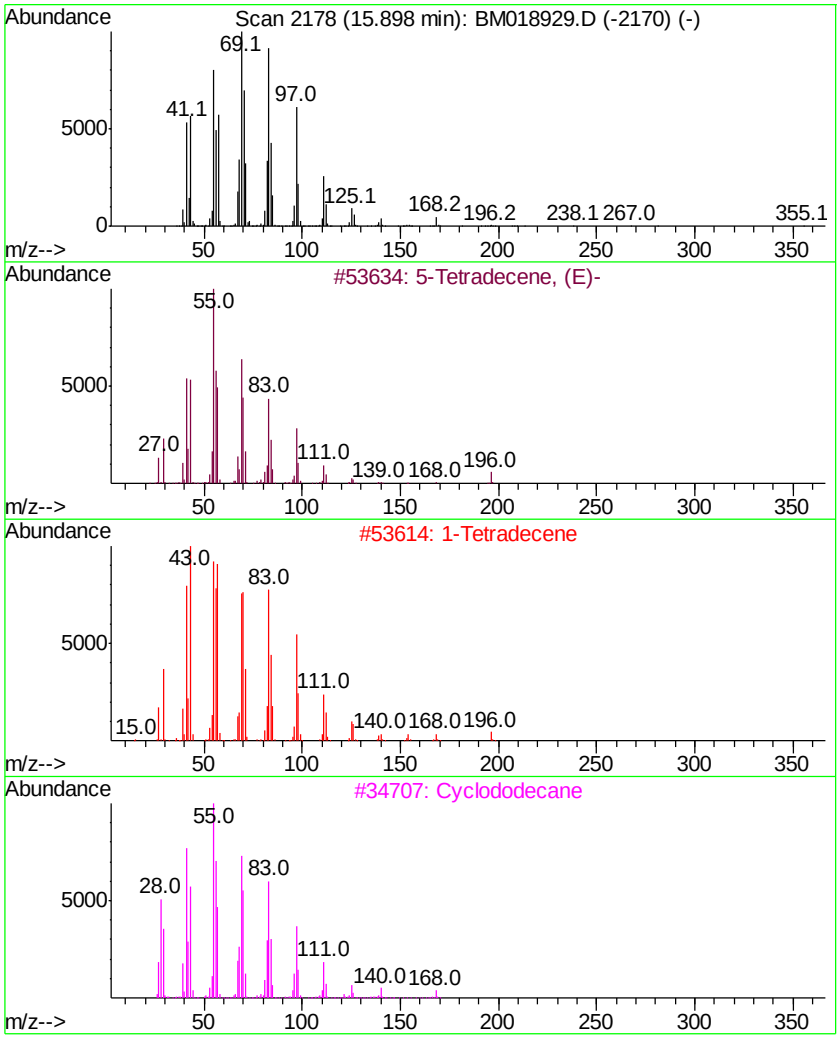
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

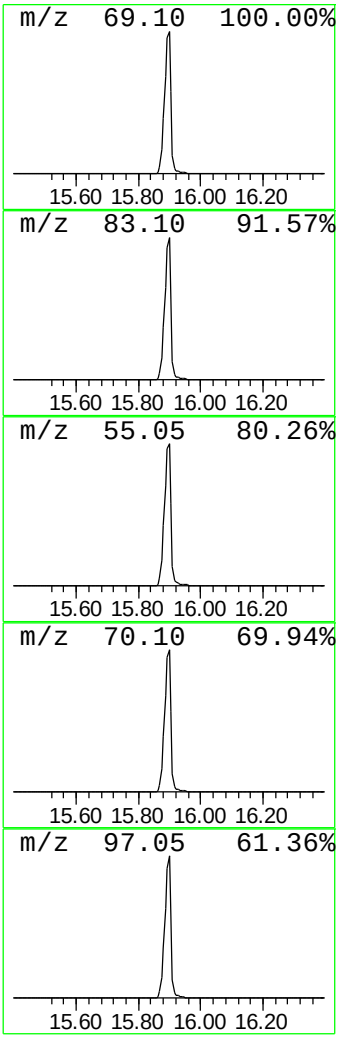
****

Peak Number 9 5-Tetradecene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.90	465.58 ng	58898100	Phenanthrene-d10	17.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Tetradecene, (E)-	196	C14H28	041446-66-6	96
2	1-Tetradecene	196	C14H28	001120-36-1	94
3	Cyclododecane	168	C12H24	000294-62-2	91
4	1-Hexadecanol	242	C16H34O	036653-82-4	91
5	3-Tetradecene, (Z)-	196	C14H28	041446-67-7	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
Data File : BM018929.D
Acq On : 26 Feb 2019 14:56
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-022019

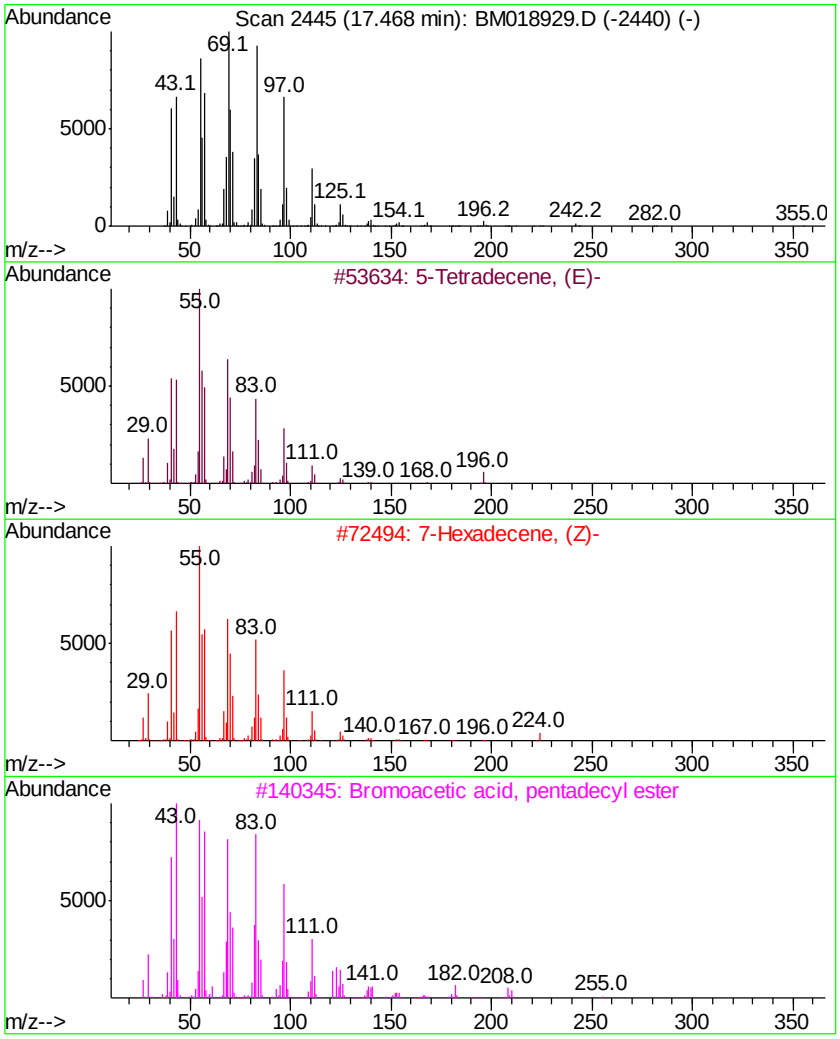
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

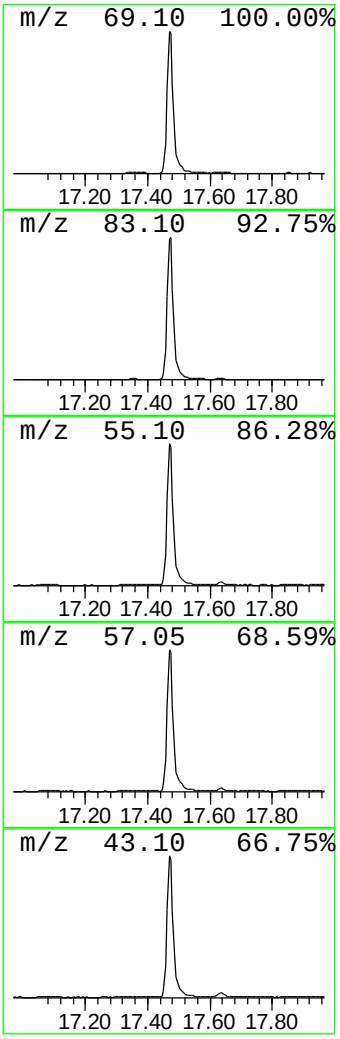
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 7-Hexadecene, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.47	109.20 ng	13813600	Phenanthrene-d10	17.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Tetradecene, (E)-	196	C14H28	041446-66-6	95
2	7-Hexadecene, (Z)-	224	C16H32	035507-09-6	93
3	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	91
4	9-Octadecene, (E)-	252	C18H36	007206-25-9	91
5	3-Hexadecene, (Z)-	224	C16H32	034303-81-6	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
Data File : BM018929.D
Acq On : 26 Feb 2019 14:56
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

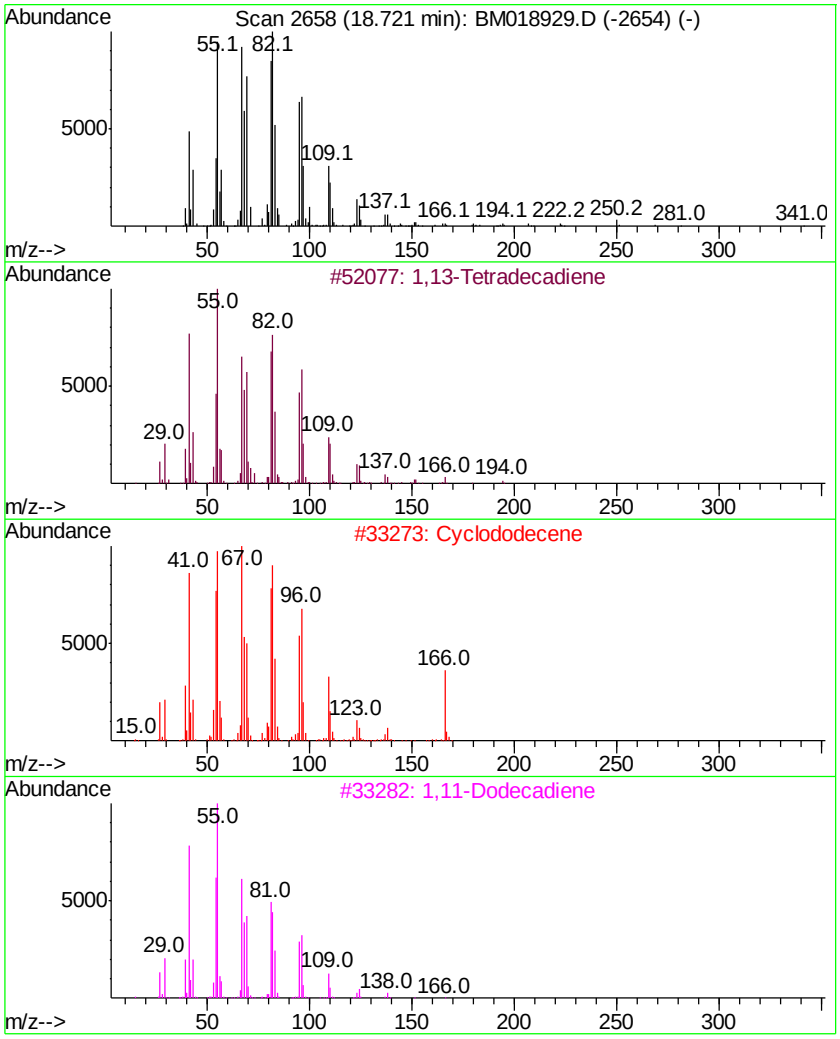
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

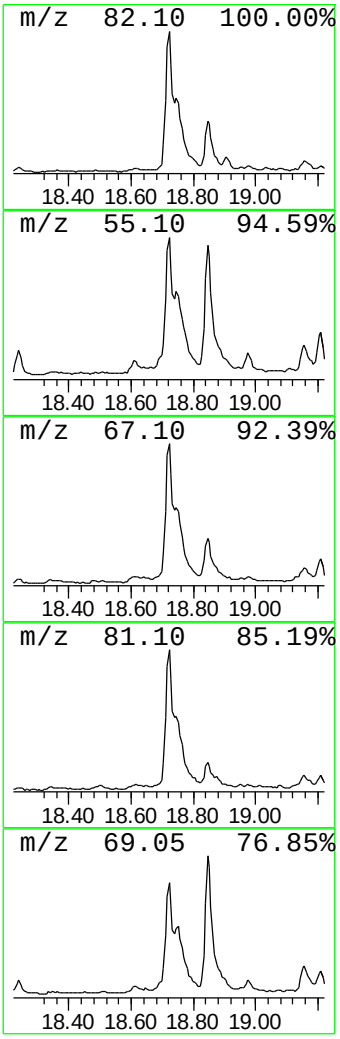
****

Peak Number 11 1,13-Tetradecadiene Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.72	9.73 ng	1230320	Phenanthrene-d10	17.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,13-Tetradecadiene	194	C14H26	021964-49-8	91
2	Cyclododecene	166	C12H22	001501-82-2	90
3	1,11-Dodecadiene	166	C12H22	005876-87-9	90
4	Z-1,6-Tridecadiene	180	C13H24	1000130-98-3	89
5	1,12-Tridecadiene	180	C13H24	021964-48-7	78





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
Data File : BM018929.D
Acq On : 26 Feb 2019 14:56
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

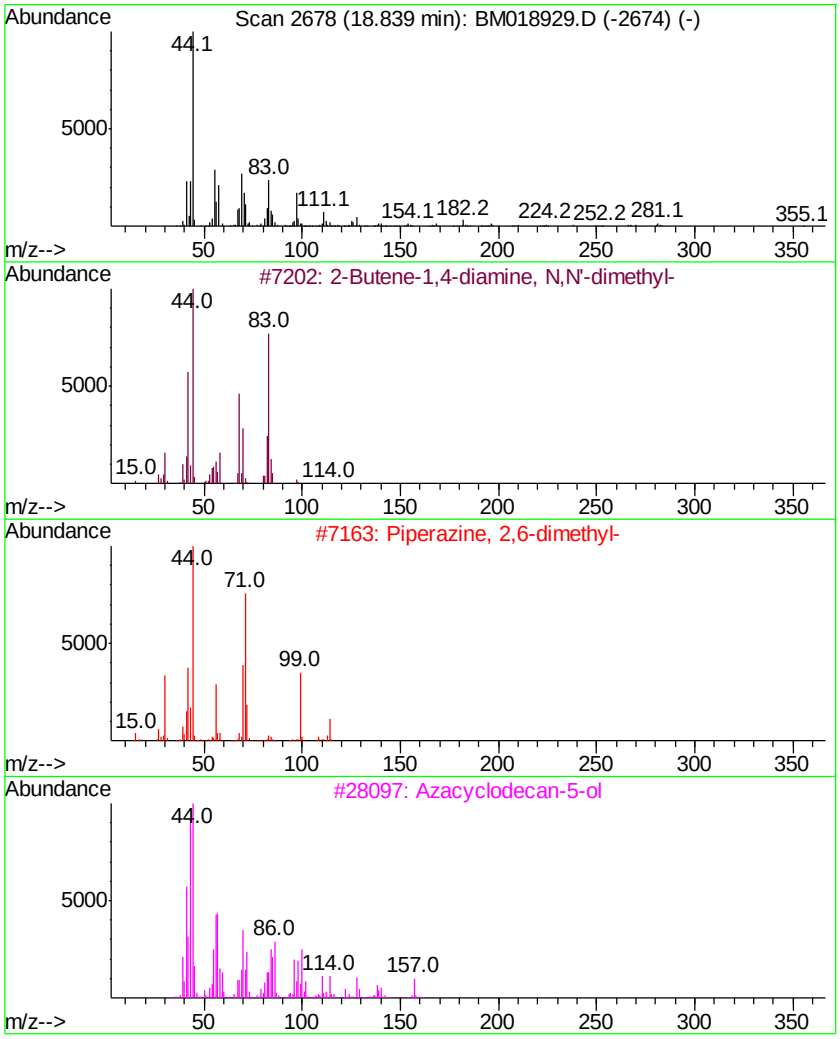
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

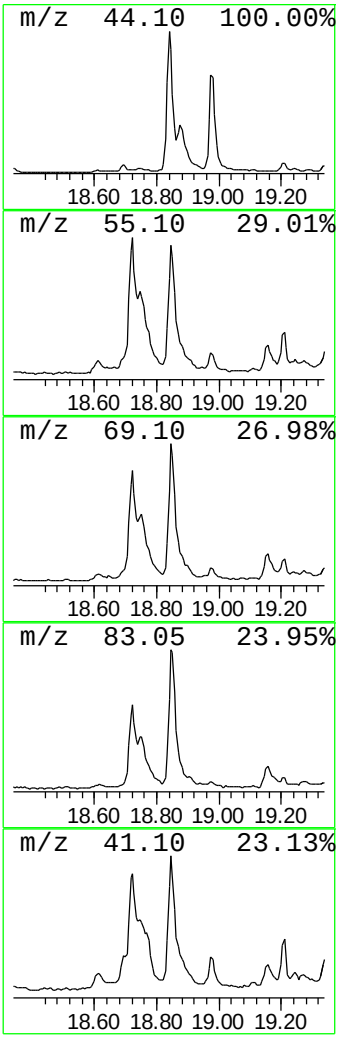
****

Peak Number 12 unknown18.84 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.84	21.56 ng	2727510	Phenanthrene-d10	17.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene-1,4-diamine, N,N'-dimet...	114	C6H14N2	000111-72-8	40
2	Piperazine, 2,6-dimethyl-	114	C6H14N2	000108-49-6	23
3	Azacyclodecan-5-ol	157	C9H19NO	1000294-90-0	23
4	3,3-Dimethyl-4-methylamino-butan...	129	C7H15NO	123528-99-4	23
5	Benzeneethanamine, 4-chloro-.alp...	169	C9H12ClN	000064-12-0	22





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
Data File : BM018929.D
Acq On : 26 Feb 2019 14:56
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

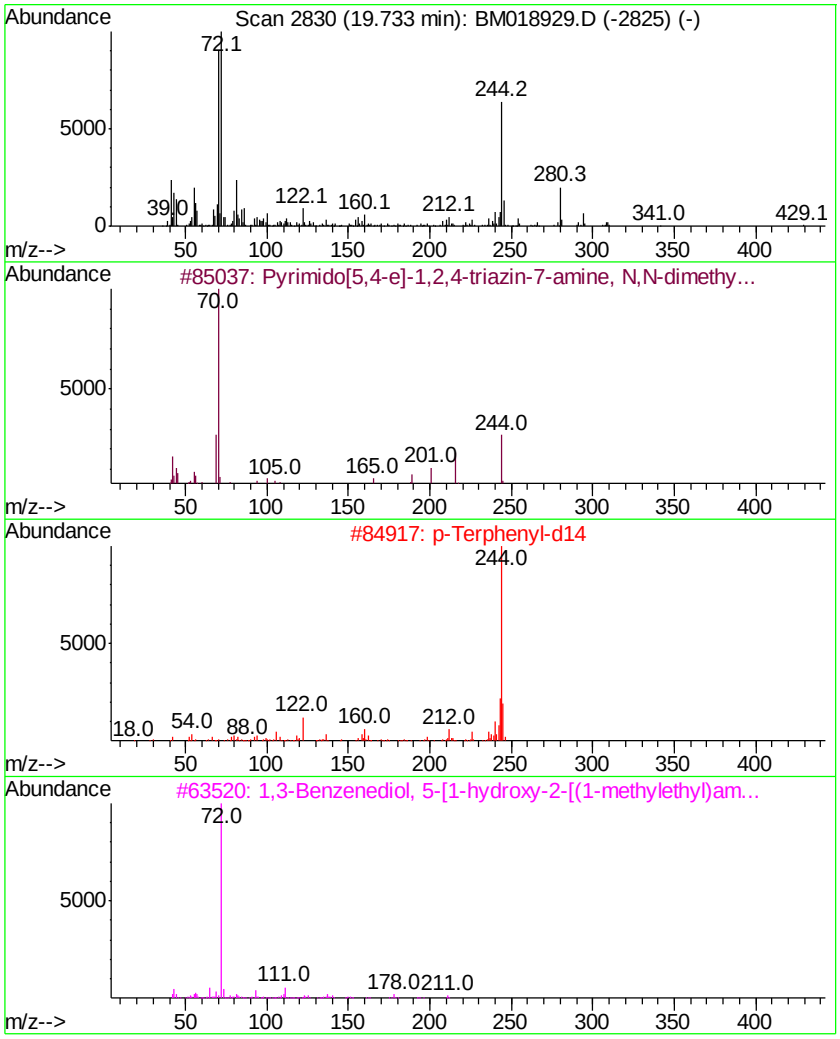
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

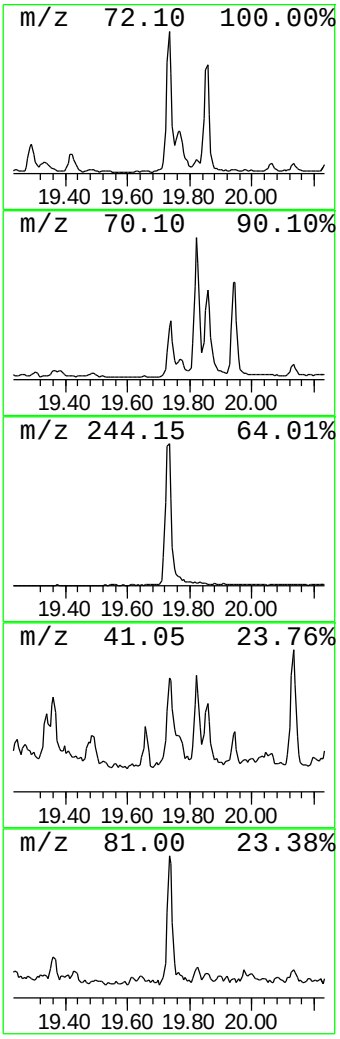
****

Peak Number 13 unknown19.73 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.73	6.95 ng	1304440	Chrysene-d12	21.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrimido[5,4-e]-1,2,4-triazin-7-...	244	C8H7F3N6	032709-26-5	38
2	p-Terphenyl-d14	244	C18D14	001718-51-0	25
3	1,3-Benzenediol, 5-[1-hydroxy-2-...	211	C11H17NO3	000586-06-1	18
4	N,N'-Diisopropylethylenediamine	144	C8H20N2	004013-94-9	14
5	(1-Ethyl-2-methylpropyl)methylamine	115	C7H17N	1000195-05-6	14





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
Data File : BM018929.D
Acq On : 26 Feb 2019 14:56
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

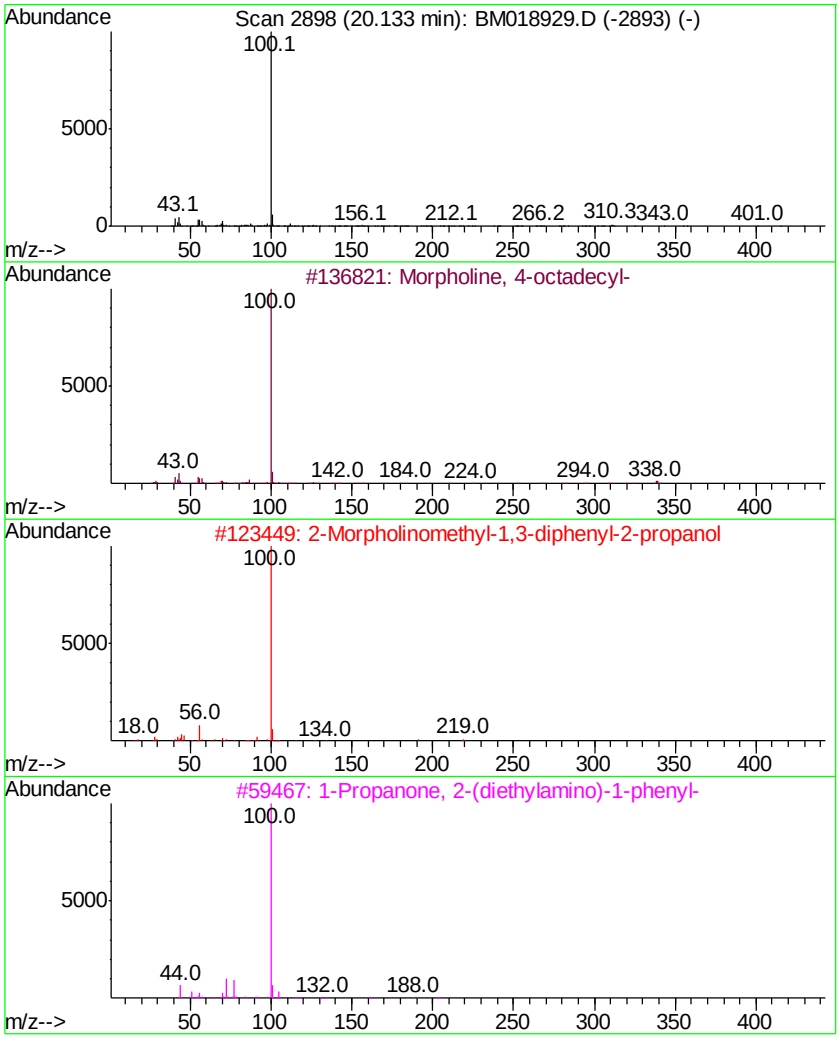
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

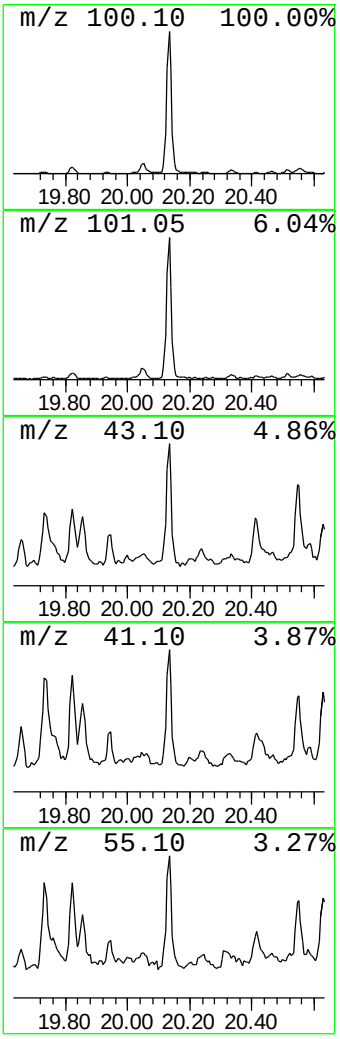
****

Peak Number 14 2-Morpholinomethyl-1,3-diph... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.13	7.94 ng	1490540	Chrysene-d12	21.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-octadecyl-	339	C22H45NO	016528-77-1	72
2	2-Morpholinomethyl-1,3-diphenyl-...	311	C20H25NO2	1000240-36-2	50
3	1-Propanone, 2-(diethylamino)-1-...	205	C13H19NO	000090-84-6	50
4	Furaltadone	324	C13H16N4O6	000139-91-3	39
5	N,N'-(O-Phenylenebis(oxytrimethy...	308	C16H24N2O4	1000244-95-1	39





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
Data File : BM018929.D
Acq On : 26 Feb 2019 14:56
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

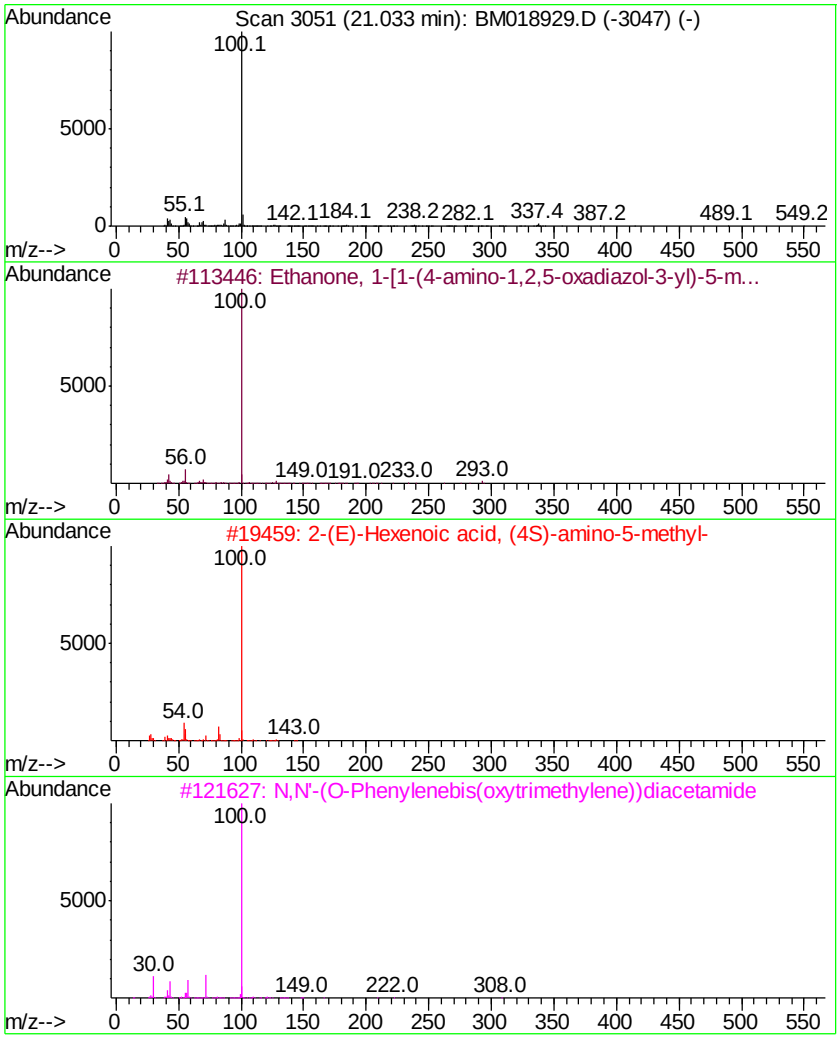
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

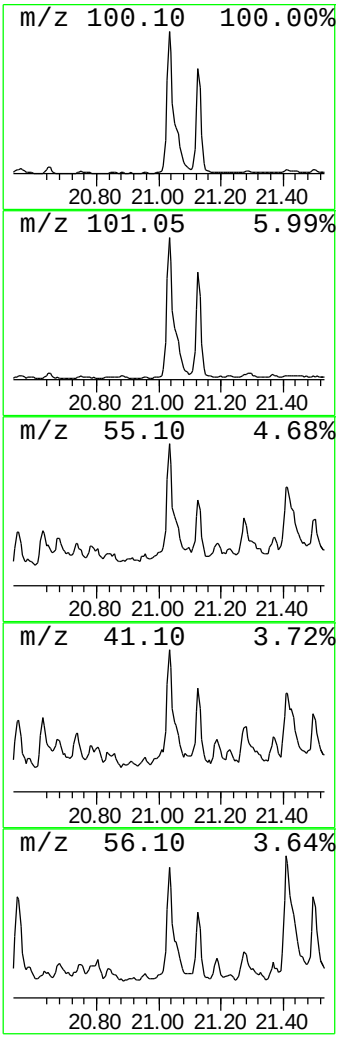
****

Peak Number 15 Ethanone, 1-[1-(4-amino-1,2... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.03	13.17 ng	2471510	Chrysene-d12	21.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-[1-(4-amino-1,2,5-ox...	293	C11H15N7O3	1000276-24-8	50
2	2-(E)-Hexenoic acid, (4S)-amino-...	143	C7H13NO2	267008-79-7	39
3	N,N'-(O-Phenylenebis(oxytrimethy...	308	C16H24N2O4	1000244-95-1	39
4	1,4-Bis(morpholinoacetyl)piperazine	340	C16H28N4O4	022764-36-9	39
5	4,9-Decadien-2-amine, N-butyl-	209	C14H27N	062238-25-9	39





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
Data File : BM018929.D
Acq On : 26 Feb 2019 14:56
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

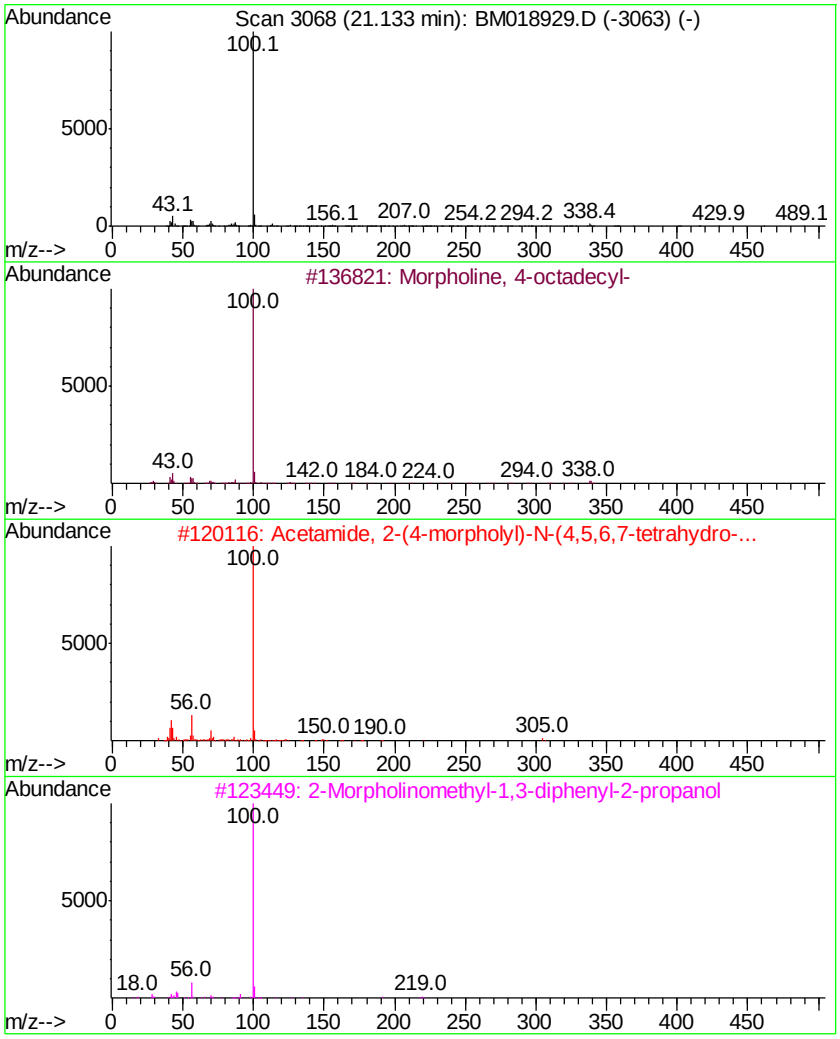
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

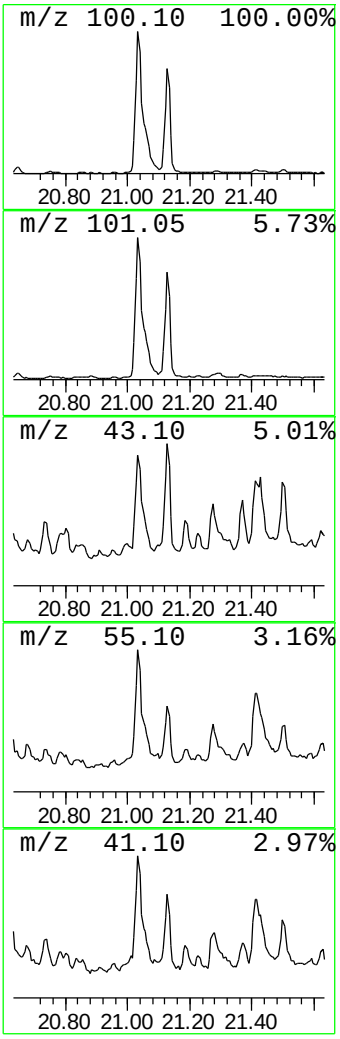
****

Peak Number 16 Morpholine, 4-octadecyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.13	6.84 ng	1283200	Chrysene-d12	21.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-octadecyl-	339	C22H45NO	016528-77-1	90
2	Acetamide, 2-(4-morpholyl)-N-(4,...	305	C15H19N3O2S	330637-98-4	50
3	2-Morpholinomethyl-1,3-diphenyl-...	311	C20H25NO2	1000240-36-2	50
4	1-[p-Nitrophenyl]-3-[2-morpholin...	294	C13H18N4O4	1000253-35-4	40
5	Tetrazole-5-(4H)-thione, 1-benzy...	291	C13H17N5OS	298687-97-5	40





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
Data File : BM018929.D
Acq On : 26 Feb 2019 14:56
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

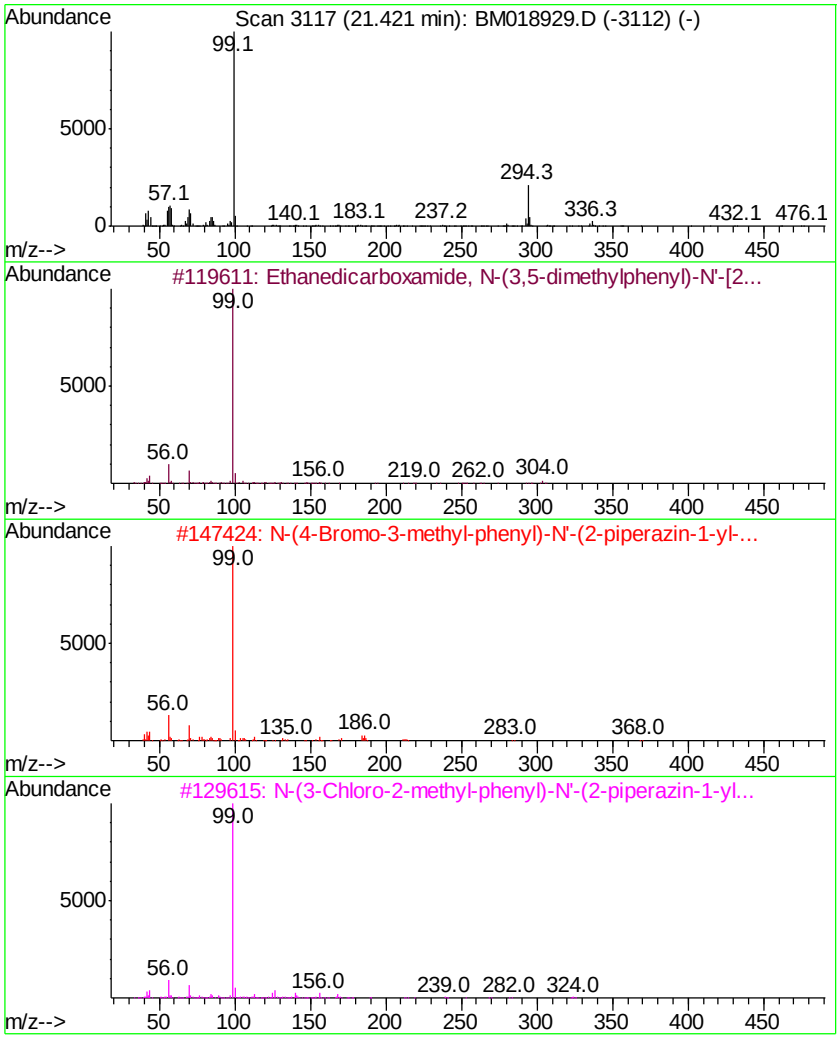
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

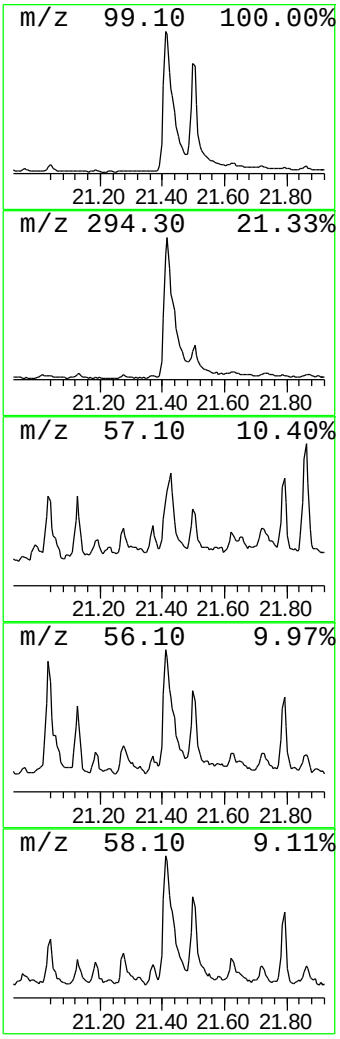
****

Peak Number 17 Ethanedicarboxamide, N-(3,5... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.42	10.16 ng	1906430	Chrysene-d12	21.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanedicarboxamide, N-(3,5-dime...	304	C16H24N4O2	346596-53-0	50
2	N-(4-Bromo-3-methyl-phenyl)-N'-(...	368	C15H21BrN4O2	1000294-59-4	50
3	N-(3-Chloro-2-methyl-phenyl)-N'-...	324	C15H21ClN4O2	1000294-79-6	50
4	N-Phenyl-N'-(2-piperazin-1-yl-et...	276	C14H20N4O2	332404-00-9	50
5	2,5-Pyrrolidinedione	99	C4H5NO2	000123-56-8	47





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
Data File : BM018929.D
Acq On : 26 Feb 2019 14:56
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

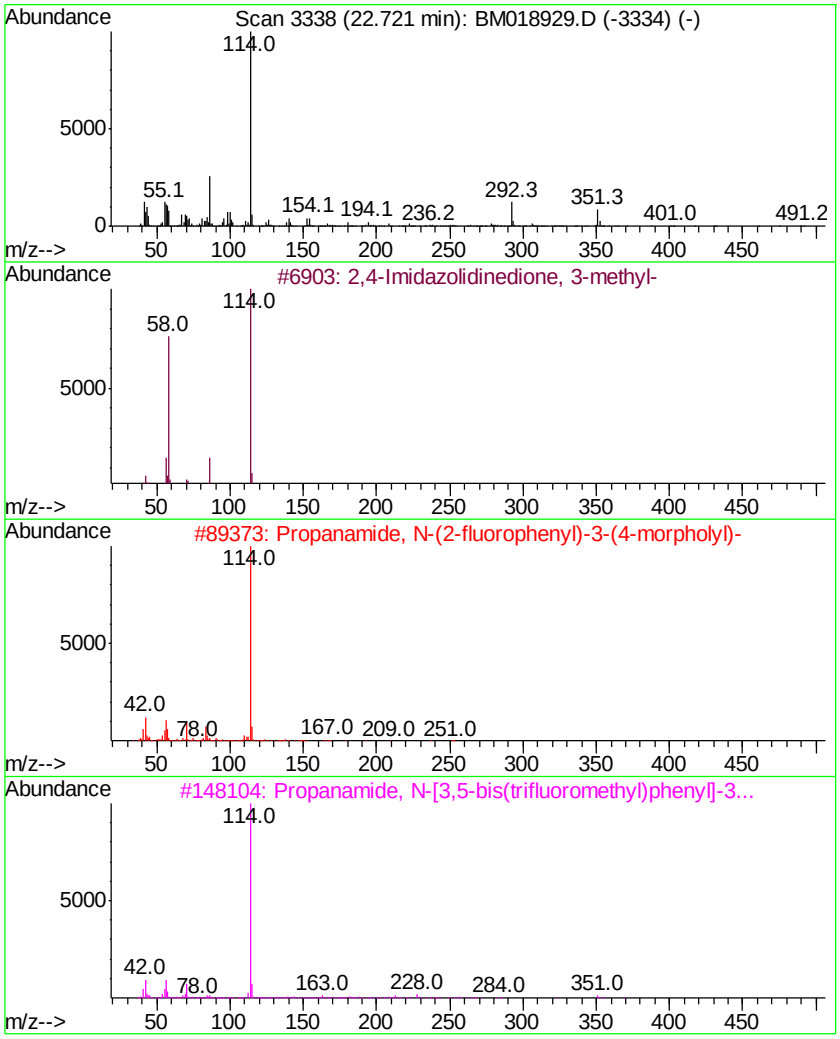
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

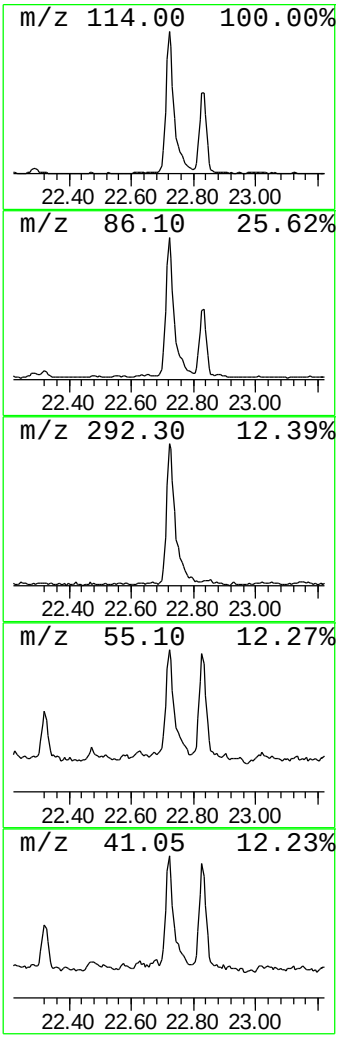
****

Peak Number 18 2,4-Imidazolidinedione, 3-m... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.72	14.25 ng	2161020	Perylene-d12	23.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Imidazolidinedione, 3-methyl-	114	C4H6N2O2	006843-45-4	53
2	Propanamide, N-(2-fluorophenyl)-...	252	C13H17FN2O2	284679-89-6	47
3	Propanamide, N-[3,5-bis(trifluor...	370	C15H16F6N2O2	1000268-58-0	47
4	DL-Threonine, N-glycyl-	176	C6H12N2O4	027174-15-8	47
5	1-Propanamine, N,N-dipropyl-	143	C9H21N	000102-69-2	45





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
Data File : BM018929.D
Acq On : 26 Feb 2019 14:56
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

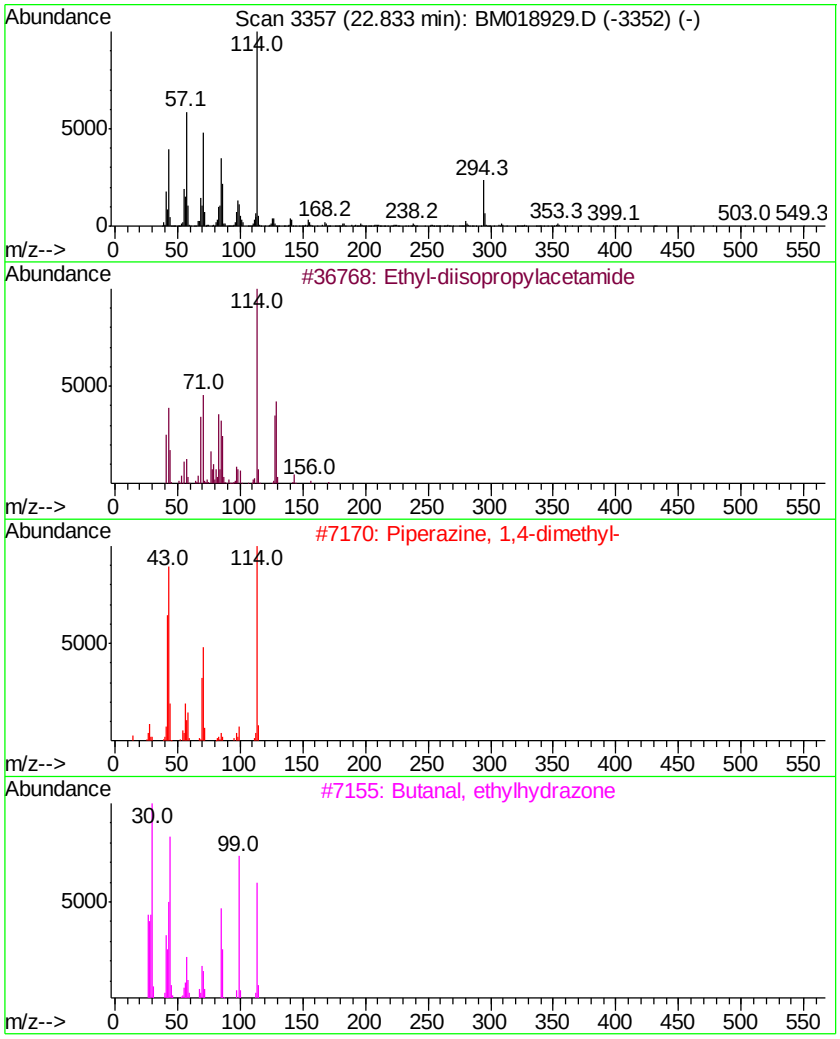
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

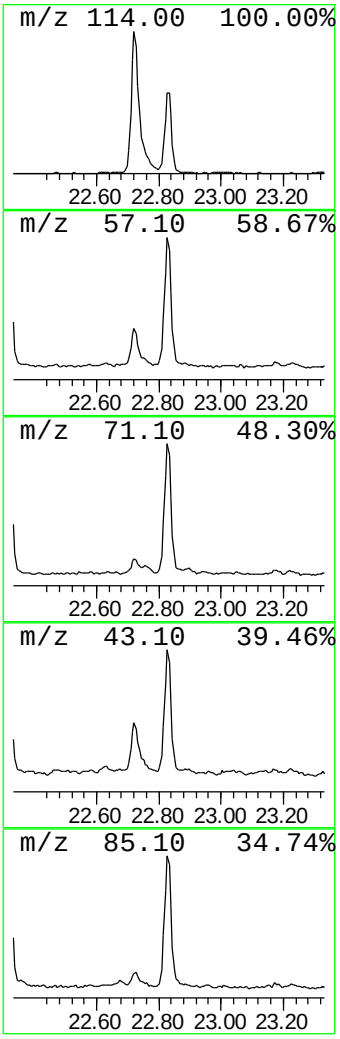
****

Peak Number 19 Ethyl-diisopropylacetamide Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.83	10.61 ng	1607920	Perylene-d12	23.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl-diisopropylacetamide	171	C10H21NO	007498-51-3	50
2	Piperazine, 1,4-dimethyl-	114	C6H14N2	000106-58-1	49
3	Butanal, ethylhydrazone	114	C6H14N2	051576-30-8	43
4	2,5-Piperazinedione	114	C4H6N2O2	000106-57-0	38
5	1,1-Di(isobutyl)acetone	170	C11H22O	040264-43-5	35





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
Data File : BM018929.D
Acq On : 26 Feb 2019 14:56
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

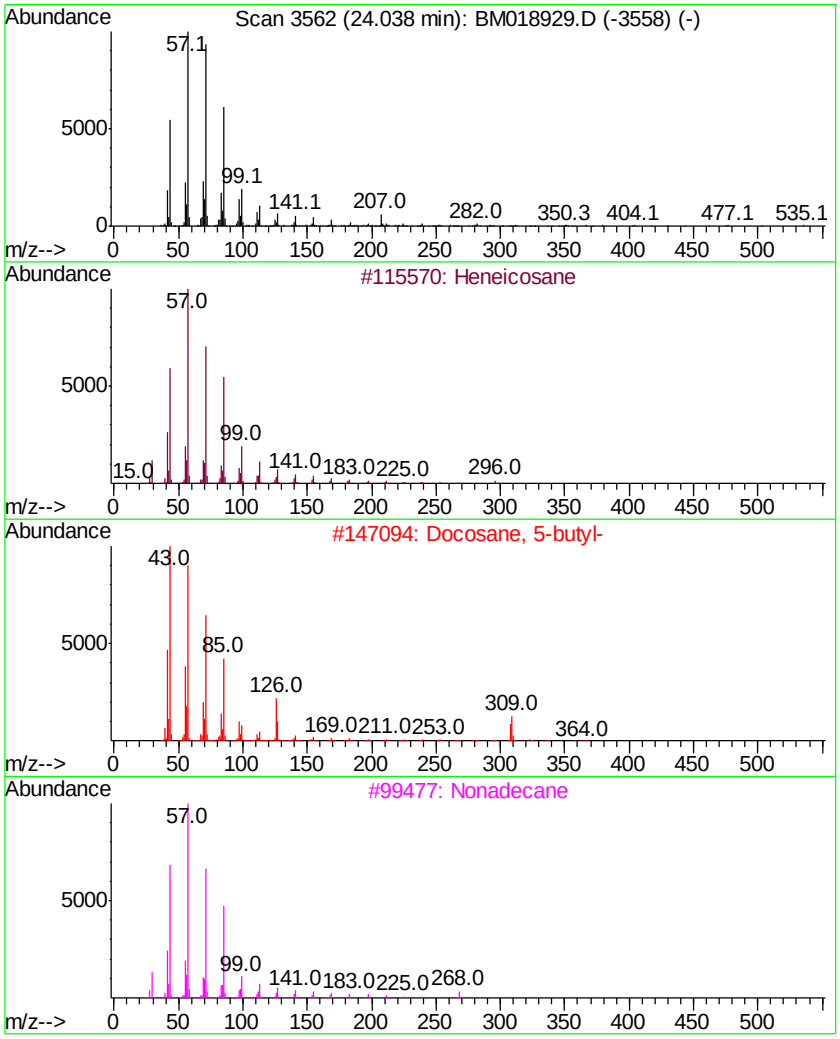
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

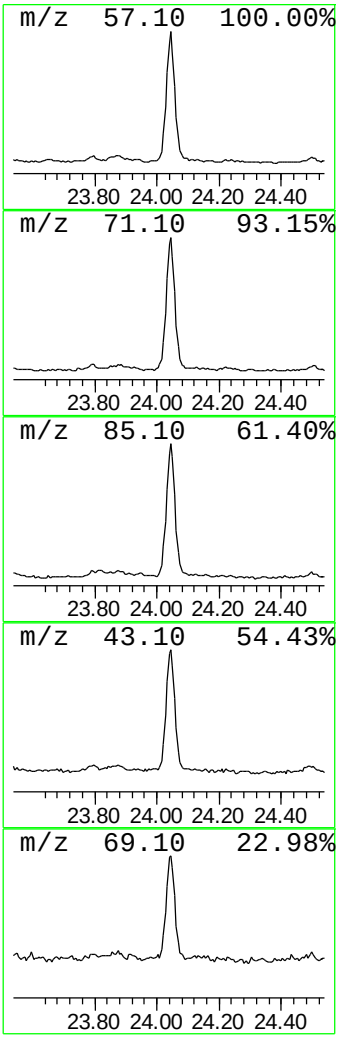
****

Peak Number 20 Heneicosane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.04	8.39 ng	1272540	Perylene-d12	23.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Docosane, 5-butyl-	366	C26H54	055282-16-1	90
3	Nonadecane	268	C19H40	000629-92-5	86
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
5	Octadecane	254	C18H38	000593-45-3	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM022619\
Data File : BM018929.D
Acq On : 26 Feb 2019 14:56
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Propanol, 1-(2-...	7.23	17.2	ng	1267790	1	7.69	1471230	20.0
2-Propanol, 1-(2-...	7.47	23.5	ng	1730750	1	7.69	1471230	20.0
3-Heptene, 2-meth...	10.32	12.3	ng	5057680	2	10.48	8195210	20.0
1-Octanol, 3,7-di...	10.37	8.3	ng	3395140	2	10.48	8195210	20.0
3-Octene, (E)-	10.68	9.9	ng	4052850	2	10.48	8195210	20.0
Cycloheptane, met...	10.86	11.7	ng	4779540	2	10.48	8195210	20.0
Cyclooctane	11.50	17.5	ng	7162820	2	10.48	8195210	20.0
1-Decene	14.02	1002.0	ng	120285000	3	14.35	2400840	20.0
5-Tetradecene, (E)-	15.90	465.6	ng	58898100	4	17.10	2530090	20.0
7-Hexadecene, (Z)-	17.47	109.2	ng	13813600	4	17.10	2530090	20.0
1,13-Tetradecadiene	18.72	9.7	ng	1230320	4	17.10	2530090	20.0
unknown18.84	18.84	21.6	ng	2727510	4	17.10	2530090	20.0
unknown19.73	19.73	7.0	ng	1304440	5	21.29	3752320	20.0
2-Morpholinomethy...	20.13	7.9	ng	1490540	5	21.29	3752320	20.0
Ethanone, 1-[1-(4...	21.03	13.2	ng	2471510	5	21.29	3752320	20.0
Morpholine, 4-oct...	21.13	6.8	ng	1283200	5	21.29	3752320	20.0
Ethanedicarboxami...	21.42	10.2	ng	1906430	5	21.29	3752320	20.0
2,4-Imidazolidine...	22.72	14.3	ng	2161020	6	23.54	3032200	20.0
Ethyl-diisopropyl...	22.83	10.6	ng	1607920	6	23.54	3032200	20.0
Heneicosane	24.04	8.4	ng	1272540	6	23.54	3032200	20.0