LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG090816\
Data File : BG023965.D
Acq On : 8 Sep 2016 12:08
Operator : UM/SJ
Sample : H4680-27
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BH-20-12-15FT

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-BG083116.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	2.973	18	23	38	rVB	3459381	5083827	100.00%	16.000%
2	5.176	393	398	406	rBV	179750	295601	5.81%	0.930%
3	5.658	474	480	491	rBV	928544	1599828	31.47%	5.035%
4	7.279	749	756	772	rBV	1053173	1953400	38.42%	6.148%
5	7.644	811	818	830	rBV	1003863	1762996	34.68%	5.549%
6	8.114	892	898	908	rVB2	161603	272784	5.37%	0.859%
7	8.437	946	953	964	rBV	669204	1215234	23.90%	3.825%
8	9.294	1092	1099	1112	rBV	677125	1237835	24.35%	3.896%
9	10.951	1372	1381	1393	rBV	211440	411379	8.09%	1.295%
10	13.395	1787	1797	1807	rBV	1786632	2907525	57.19%	9.151%
11	14.223	1932	1938	1946	rBV	1018825	1476031	29.03%	4.645%
12	14.781	2027	2033	2040	rVB2	408065	682344	13.42%	2.148%
13	15.592	2167	2171	2175	rVB2	46572	58485	1.15%	0.184%
14	16.279	2281	2288	2303	rBV	2016871	3240834	63.75%	10.200%
15	16.455	2314	2318	2328	rVB3	55342	113301	2.23%	0.357%
16	17.254	2449	2454	2458	rBV	66415	76629	1.51%	0.241%
17	17.542	2497	2503	2509	rBV	600273	939220	18.47%	2.956%
18	17.900	2555	2564	2573	rBV8	57961	166547	3.28%	0.524%
19	17.994	2576	2580	2586	rVB2	60558	85860	1.69%	0.270%
20	18.405	2646	2650	2659	rBV5	77407	133787	2.63%	0.421%
21	18.687	2695	2698	2704	rBV2	45677	71643	1.41%	0.225%
22	19.257	2791	2795	2802	rBV2	265640	529419	10.41%	1.666%
23	20.144	2940	2946	2951	rBV	3771290	4948856	97.35%	15.575%
24	20.420	2988	2993	2997	rBV5	71159	114352	2.25%	0.360%
25	20.761	3047	3051	3059	rVB2	86639	126948	2.50%	0.400%
26	20.879	3068	3071	3074	rVV2	121150	131459	2.59%	0.414%
27	21.443	3165	3167	3179	rVB2	58355	137012	2.70%	0.431%
28	21.854	3231	3237	3247	rBV2	633760	1067661	21.00%	3.360%
29	25.243	3805	3814	3824	rVB	324881	933063	18.35%	2.937%

Sum of corrected areas: 31773860

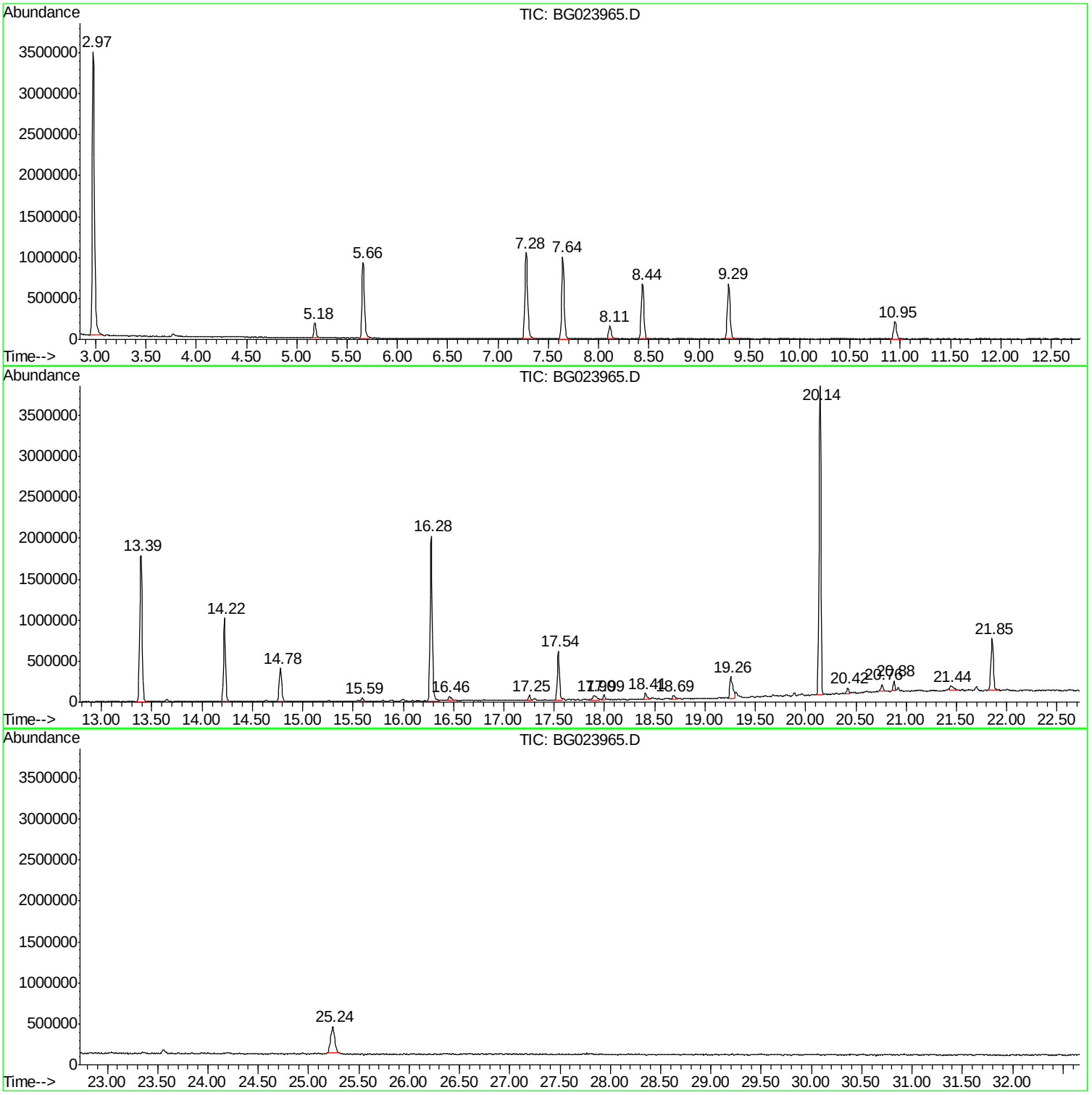
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG090816\
Data File : BG023965.D
Acq On : 8 Sep 2016 12:08
Operator : UM/SJ
Sample : H4680-27
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BH-20-12-15FT

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.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\BG090816\
Data File : BG023965.D
Acq On : 8 Sep 2016 12:08
Operator : UM/SJ
Sample : H4680-27
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BH-20-12-15FT

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

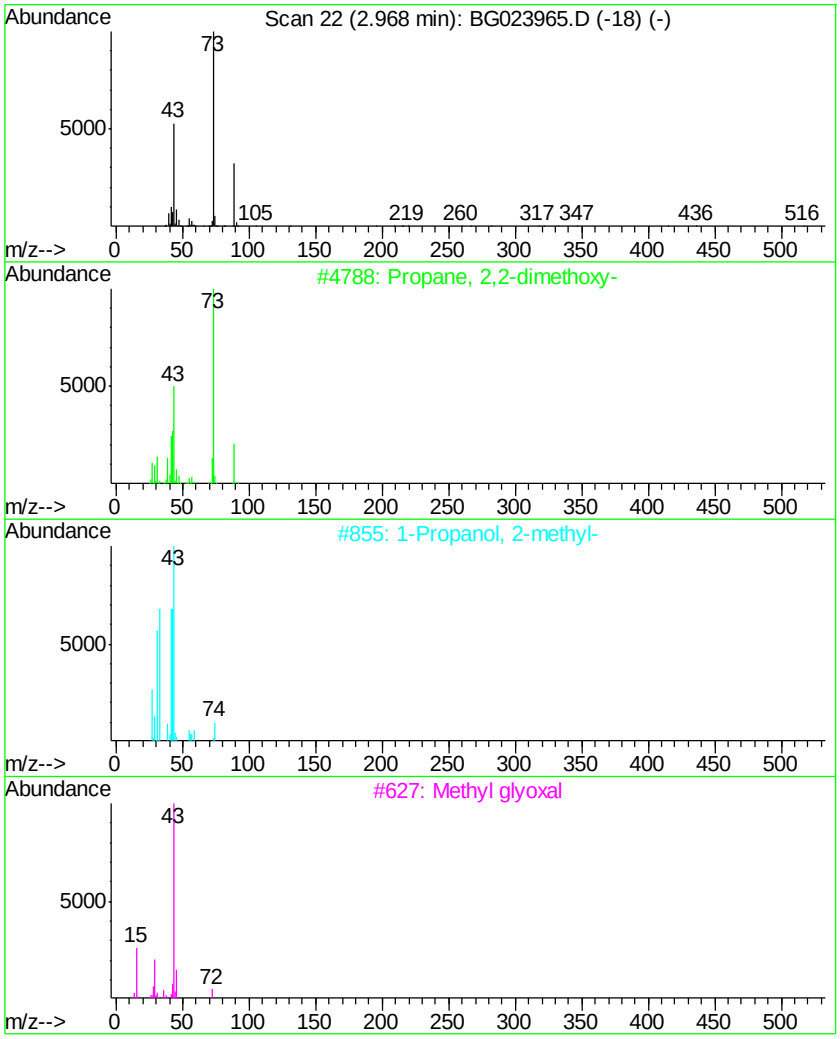
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

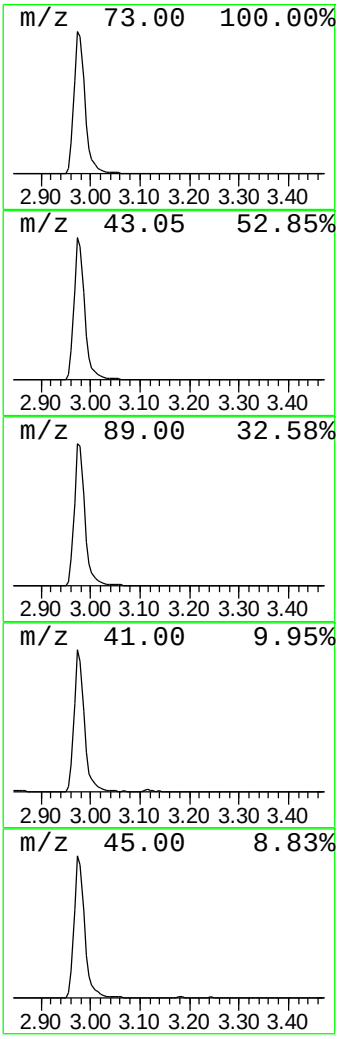
****

Peak Number 1 unknown2.97 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.97	372.74 ng	5083830	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
3	Methyl glyoxal	72	C3H4O2	000078-98-8	9
4	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG090816\
Data File : BG023965.D
Acq On : 8 Sep 2016 12:08
Operator : UM/SJ
Sample : H4680-27
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BH-20-12-15FT

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

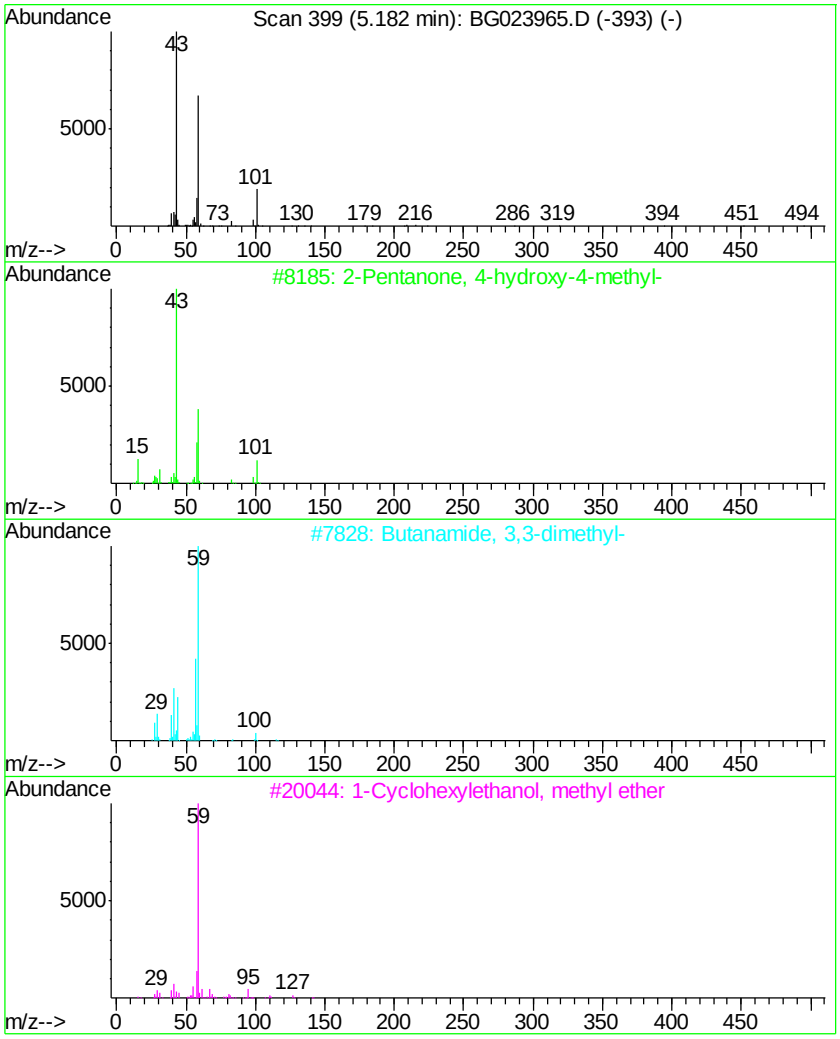
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

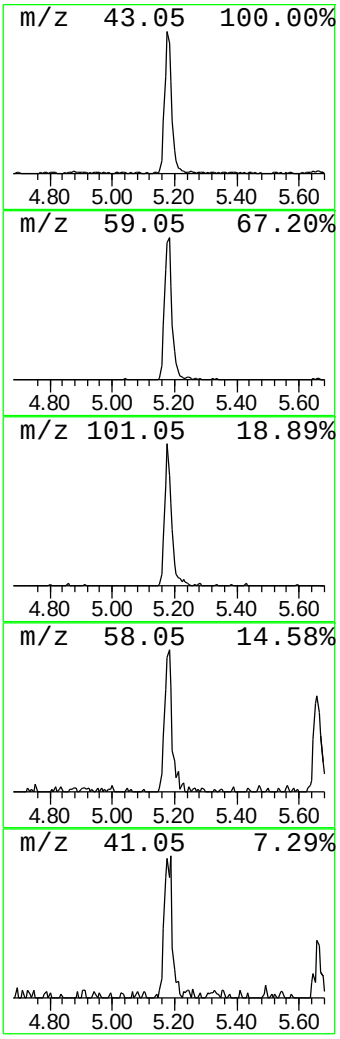
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	21.67 ng	295601	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	25
3	1-Cyclohexylethanol, methyl ether	142	C9H18O	1000365-12-8	17
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG090816\
Data File : BG023965.D
Acq On : 8 Sep 2016 12:08
Operator : UM/SJ
Sample : H4680-27
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BH-20-12-15FT

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

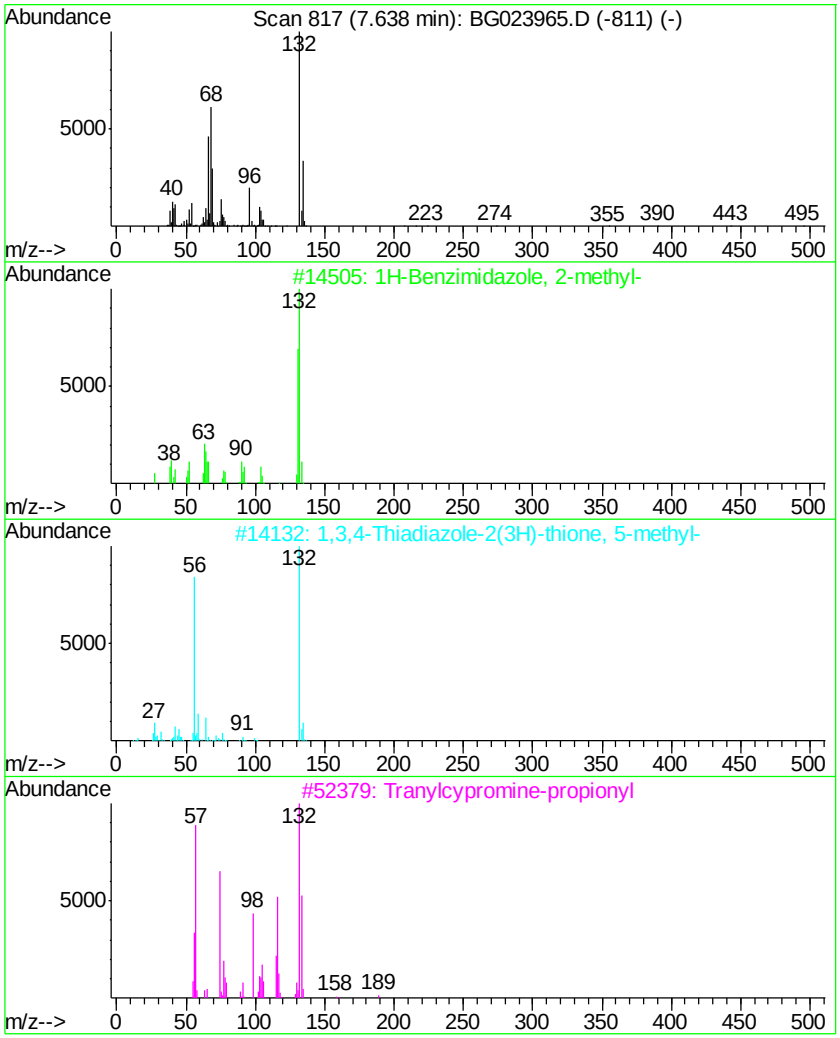
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

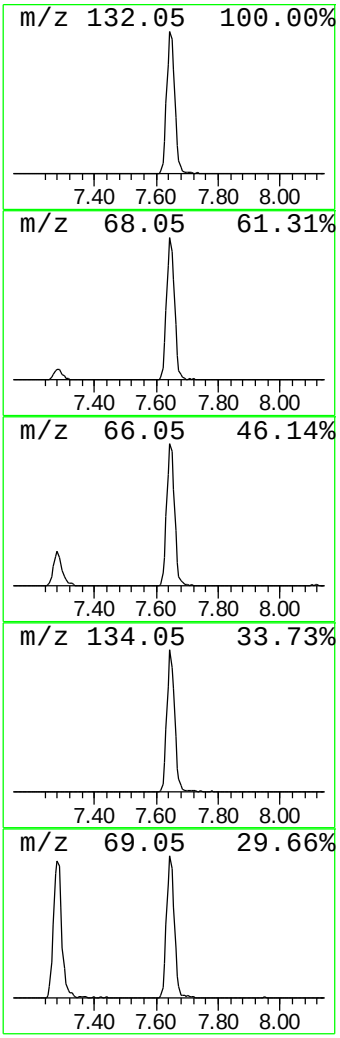
****

Peak Number 3 unknown7.64 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	129.26 ng	1763000	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	18
2	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5	Xenon	132	Xe	007440-63-3	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG090816\
Data File : BG023965.D
Acq On : 8 Sep 2016 12:08
Operator : UM/SJ
Sample : H4680-27
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BH-20-12-15FT

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

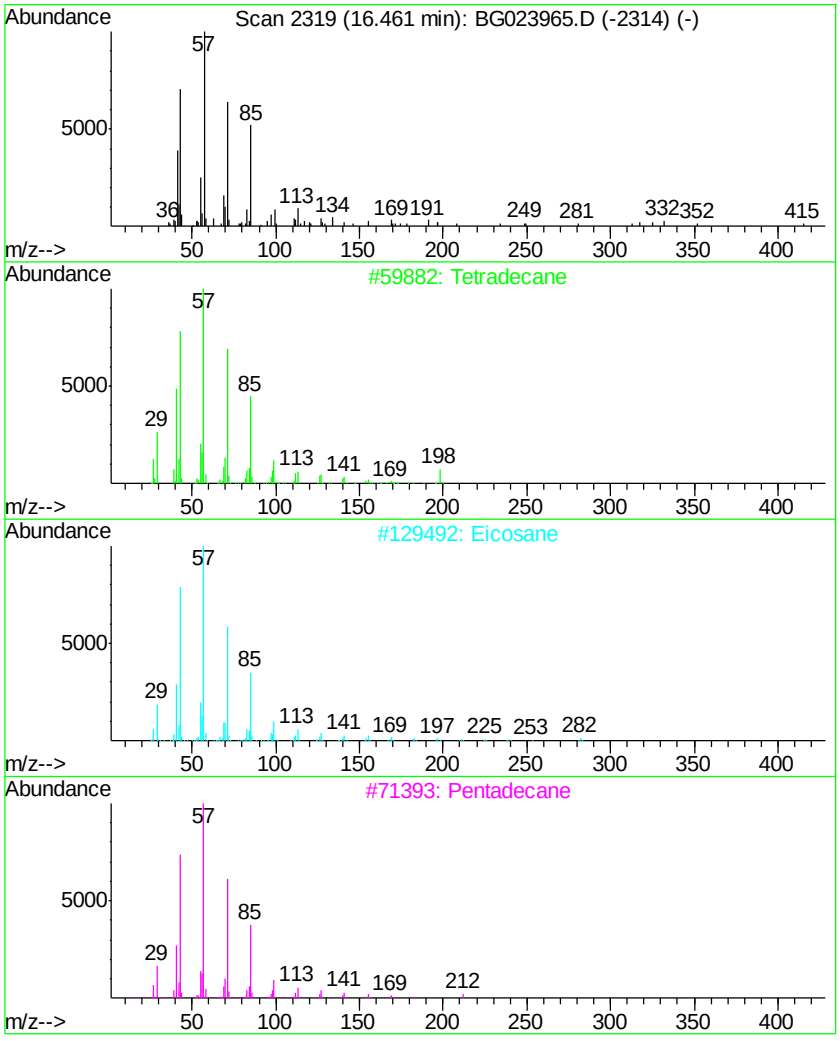
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

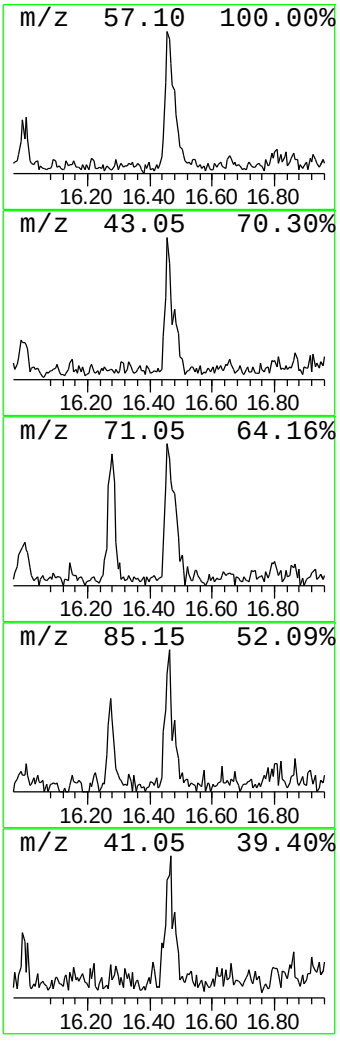
****

Peak Number 5 Tetradecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.46	2.41 ng	113301	Phenanthrene-d10	17.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	80
2	Eicosane	282	C20H42	000112-95-8	80
3	Pentadecane	212	C15H32	000629-62-9	80
4	Tridecane, 6-propyl-	226	C16H34	055045-10-8	80
5	Hexadecane	226	C16H34	000544-76-3	80





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG090816\
Data File : BG023965.D
Acq On : 8 Sep 2016 12:08
Operator : UM/SJ
Sample : H4680-27
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BH-20-12-15FT

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.M
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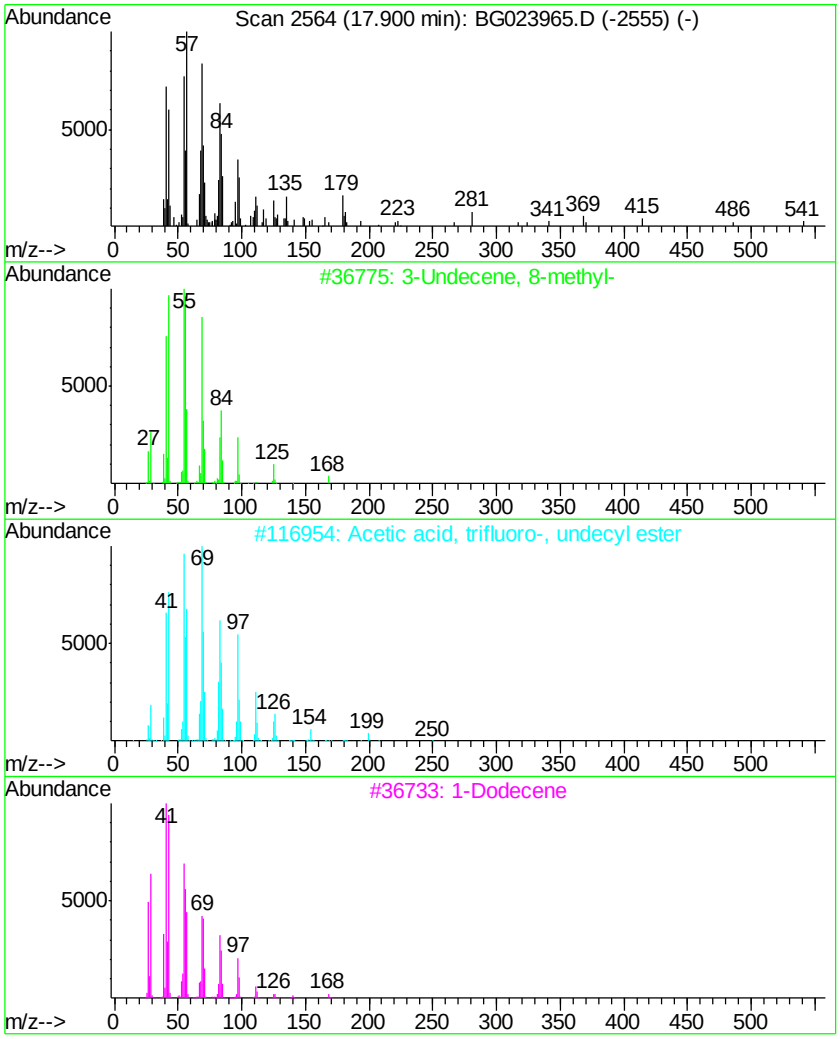
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

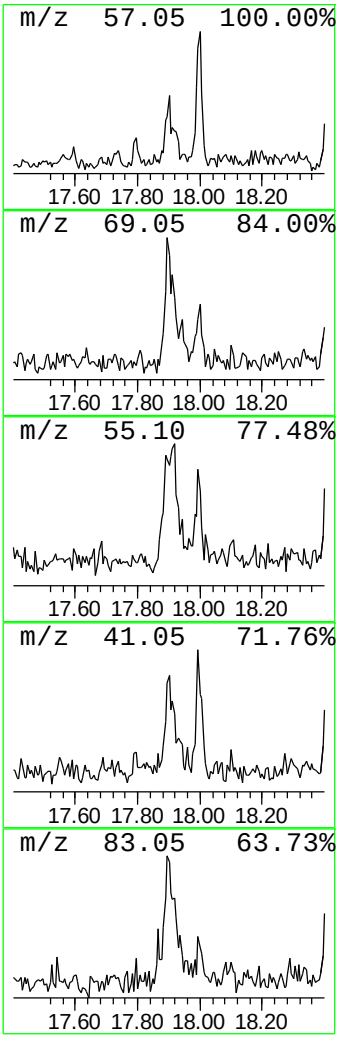
****

Peak Number 6 3-Undecene, 8-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.90	3.55 ng	166547	Phenanthrene-d10	17.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Undecene, 8-methyl-	168	C12H24	1000061-84-4	70
2	Acetic acid, trifluoro-, undecyl...	268	C13H23F3O2	053800-01-4	64
3	1-Dodecene	168	C12H24	000112-41-4	52
4	3-Hexadecene, (Z)-	224	C16H32	034303-81-6	52
5	3-Heptafluorobutyroxytetradecane	410	C18H29F7O2	1000245-49-8	52





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG090816\
Data File : BG023965.D
Acq On : 8 Sep 2016 12:08
Operator : UM/SJ
Sample : H4680-27
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BH-20-12-15FT

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

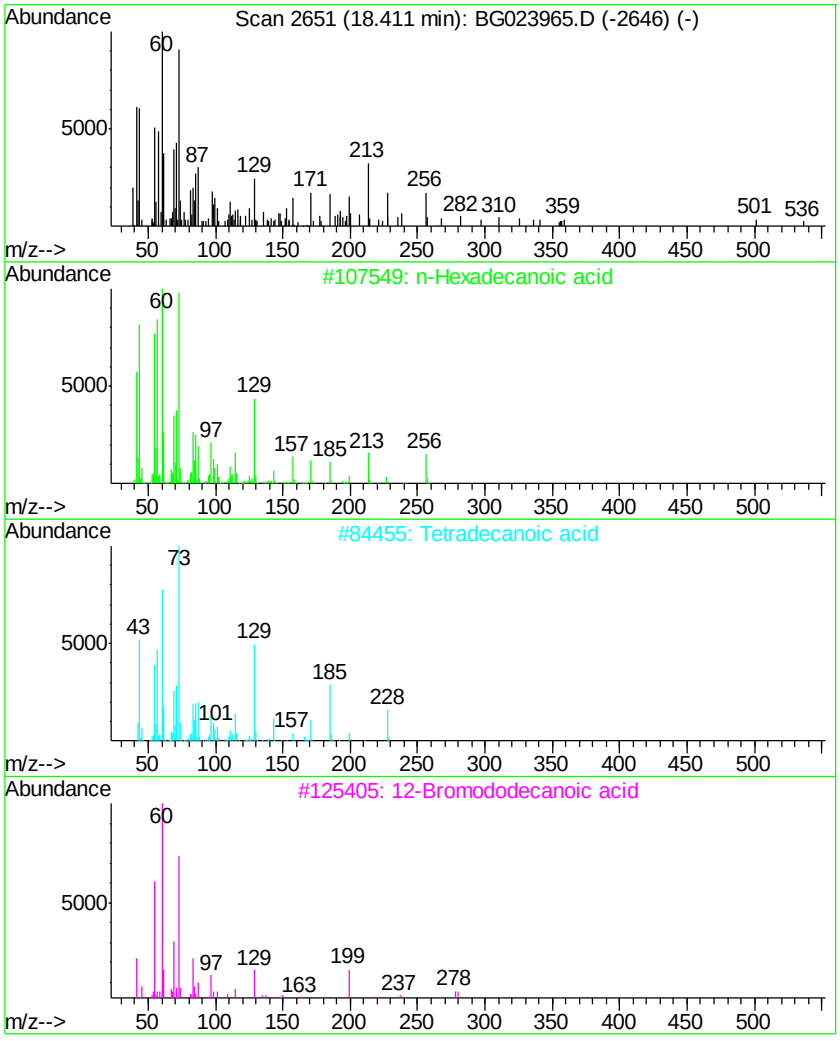
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

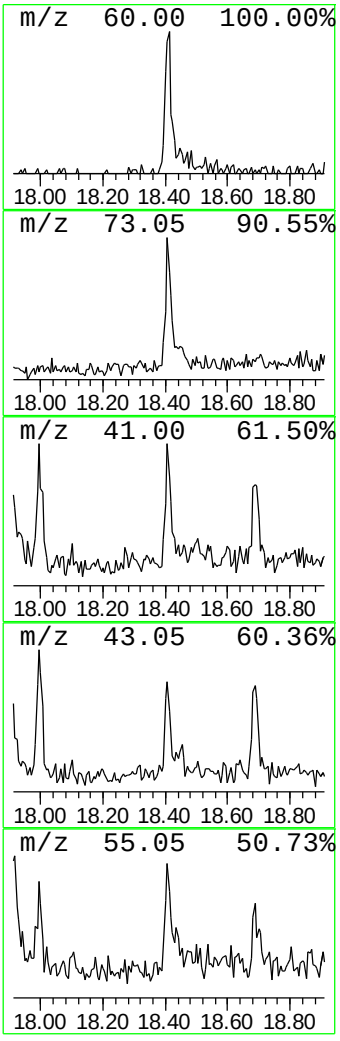
****

Peak Number 7 unknown18.41 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.41	2.85 ng	133787	Phenanthrene-d10	17.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	47
3	12-Bromododecanoic acid	278	C12H23BrO2	073367-80-3	42
4	Nonanoic acid	158	C9H18O2	000112-05-0	38
5	Dodecanoic acid	200	C12H24O2	000143-07-7	38





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG090816\
Data File : BG023965.D
Acq On : 8 Sep 2016 12:08
Operator : UM/SJ
Sample : H4680-27
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BH-20-12-15FT

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

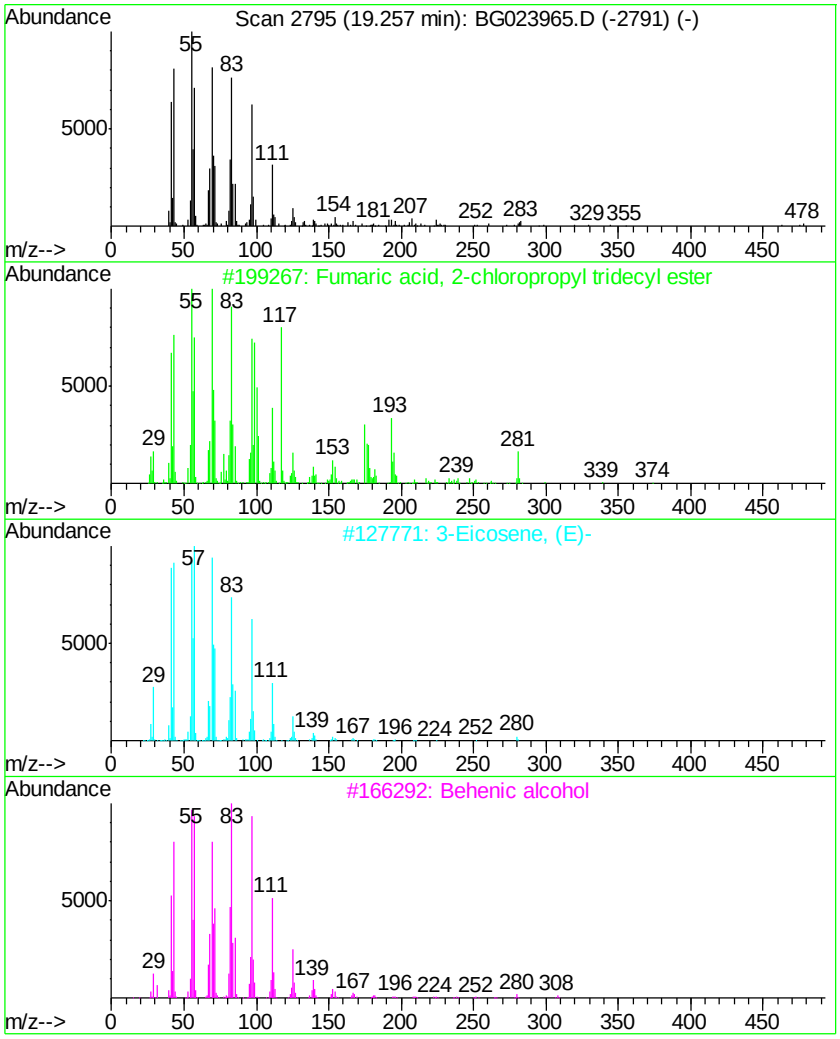
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

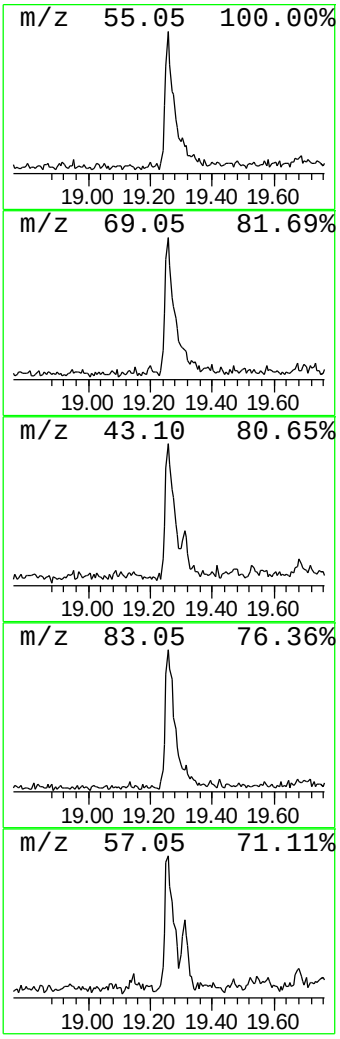
****

Peak Number 8 Fumaric acid, 2-chloropropy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.26	11.27 ng	529419	Phenanthrene-d10	17.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fumaric acid, 2-chloropropyl tri...	374	C20H35ClO4	1000348-57-1	90
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	87
3	Behenic alcohol	326	C22H46O	000661-19-8	76
4	1-Eicosanol	298	C20H42O	000629-96-9	76
5	1-Heneicosanol	312	C21H44O	015594-90-8	76





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG090816\
Data File : BG023965.D
Acq On : 8 Sep 2016 12:08
Operator : UM/SJ
Sample : H4680-27
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BH-20-12-15FT

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

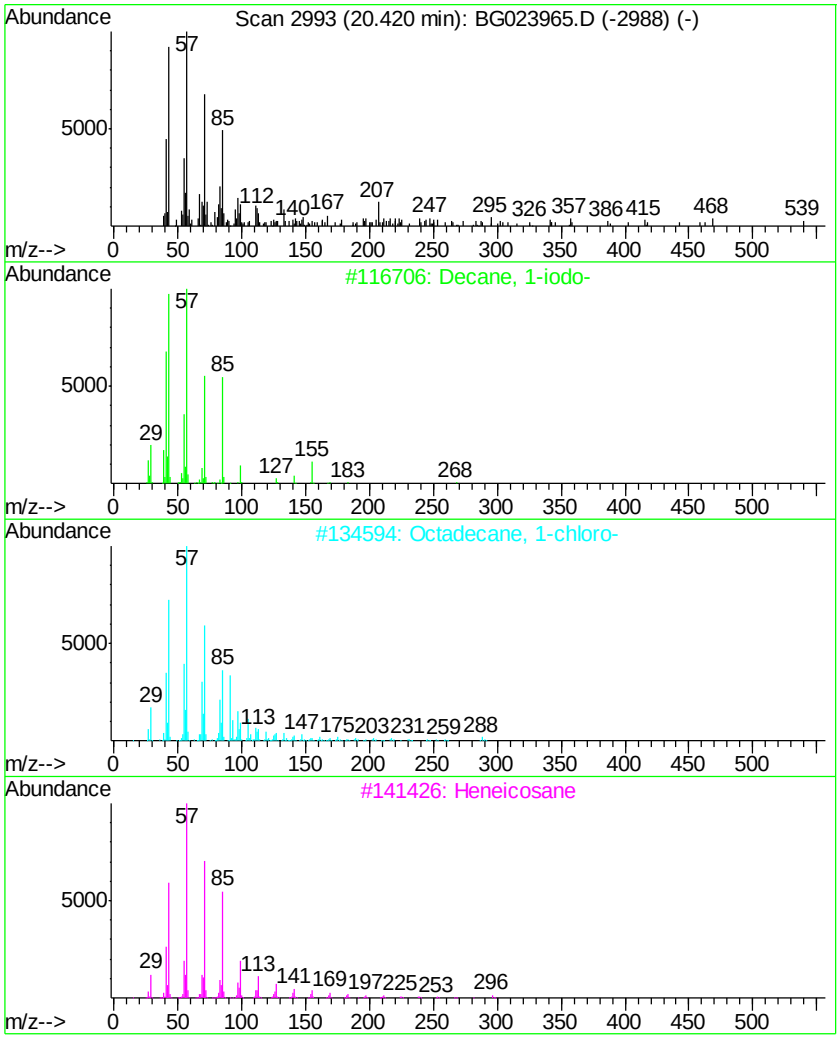
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

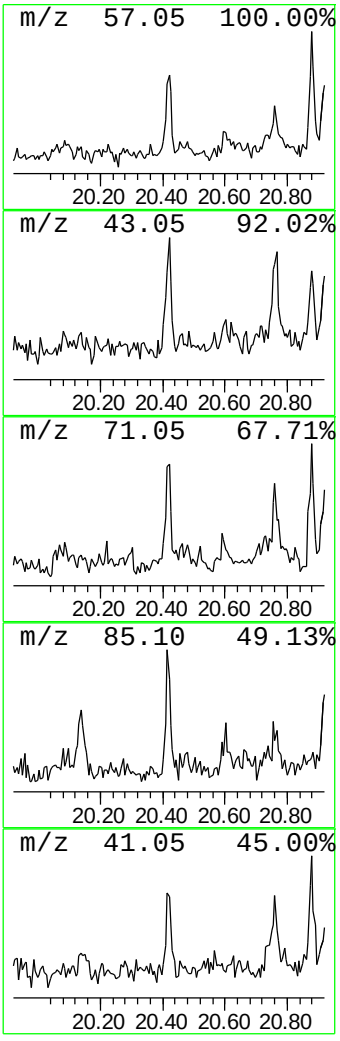
****

Peak Number 9 Decane, 1-iodo- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.42	2.14 ng	114352	Chrysene-d12	21.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 1-iodo-	268	C10H21I	002050-77-3	89
2	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	89
3	Heneicosane	296	C21H44	000629-94-7	76
4	Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	70
5	Tetratetracontane	619	C44H90	007098-22-8	68





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Data File : BG023965.D
Acq On : 8 Sep 2016 12:08
Operator : UM/SJ
Sample : H4680-27
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BH-20-12-15FT

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

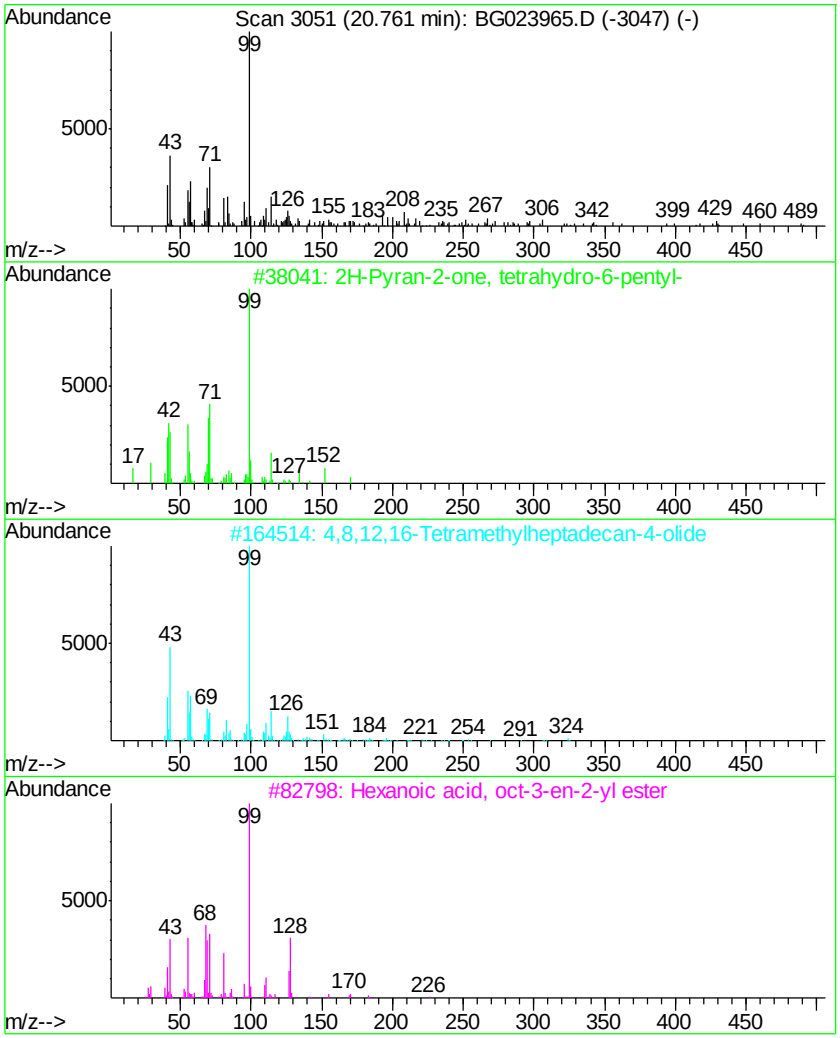
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

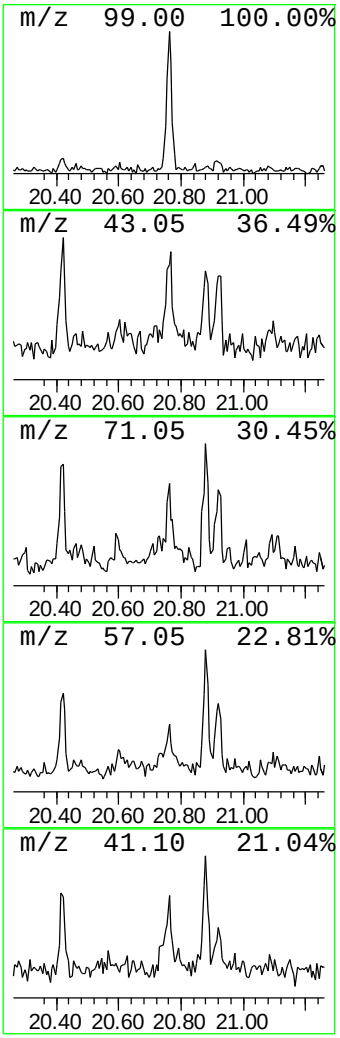
****

Peak Number 10 2H-Pyran-2-one, tetrahydro-... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.76	2.38 ng	126948	Chrysene-d12	21.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Pyran-2-one, tetrahydro-6-pen...	170	C10H18O2	000705-86-2	72
2	4,8,12,16-Tetramethylheptadecan-...	324	C21H40O2	096168-15-9	72
3	Hexanoic acid, oct-3-en-2-yl ester	226	C14H26O2	1000299-35-5	64
4	D-Gluconic acid, 1,2:3,4:5,6-tri...	310	C12H21B3O7	1000157-46-5	64
5	2H-Pyran-2-one, tetrahydro-6-octyl-	212	C13H24O2	007370-92-5	64





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG090816\
Data File : BG023965.D
Acq On : 8 Sep 2016 12:08
Operator : UM/SJ
Sample : H4680-27
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BH-20-12-15FT

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.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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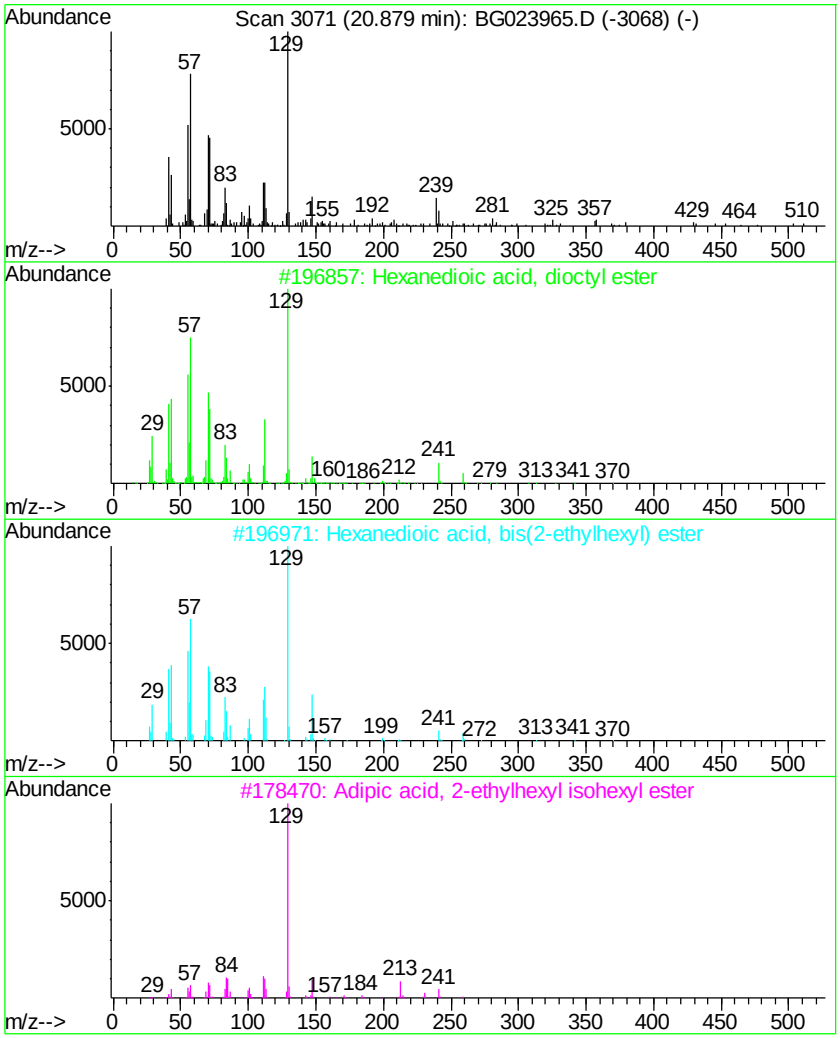
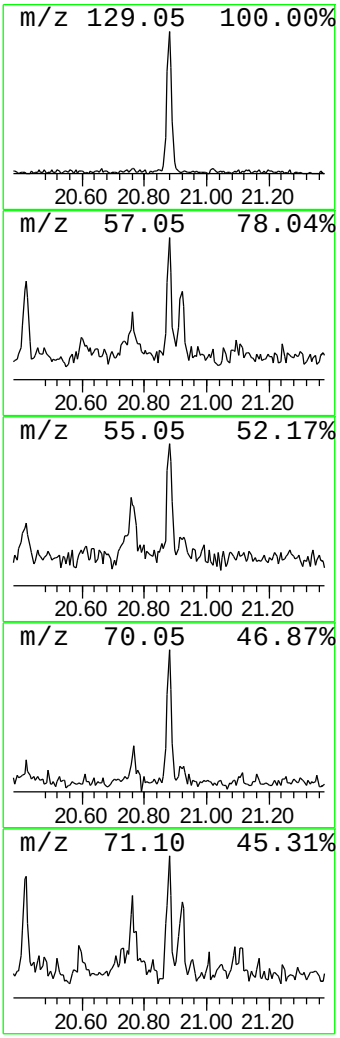
Peak Number 11 Hexanedioic acid, dioctyl e... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.88	2.46 ng	131459	Chrysene-d12	21.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	64
2	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	43
3	Adipic acid, 2-ethylhexyl isohex...	342	C20H38O4	1000324-48-3	38
4	Adipic acid, 2-methylpent-3-yl o...	342	C20H38O4	1000353-56-3	38
5	Adipic acid, isohexyl 3-pentyl e...	300	C17H32O4	1000324-60-7	27





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG090816\
Data File : BG023965.D
Acq On : 8 Sep 2016 12:08
Operator : UM/SJ
Sample : H4680-27
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BH-20-12-15FT

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.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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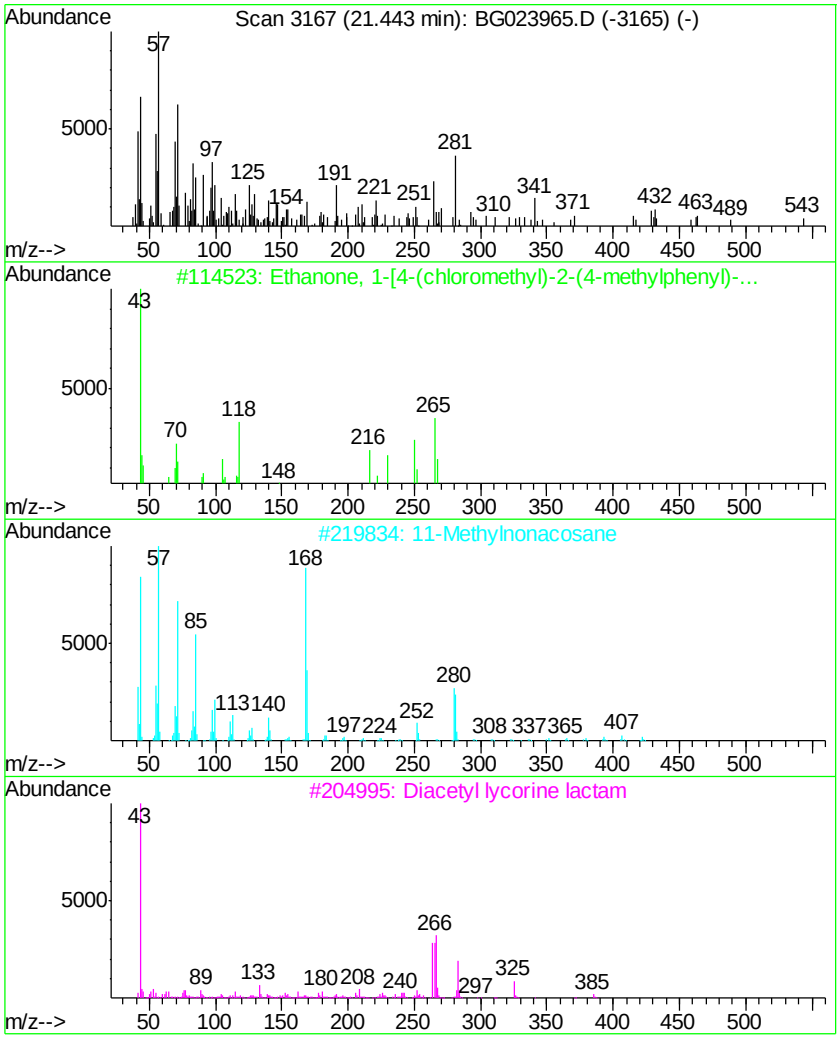
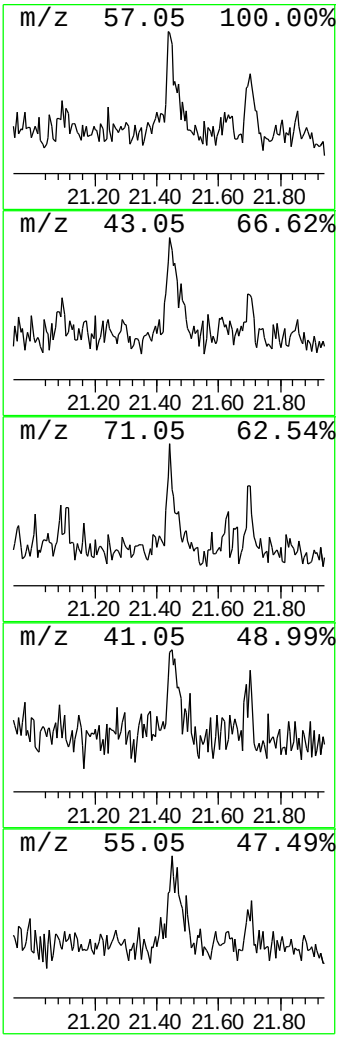
Peak Number 12 unknown21.44 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.44	2.57 ng	137012	Chrysene-d12	21.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-[4-(chloromethyl)-2-...	265	C13H12ClNOS	041991-34-8	10
2	11-Methylnonacosane	422	C30H62	007371-99-5	9
3	Diacetyl lycorine lactam	385	C20H19NO7	006391-78-2	9
4	21-Norpicrasane-20-carboxylic ac...	536	C27H36O11	076389-73-6	9
5	1H-Benzo[3,4]cyclobuta[1,2-b]pyr...	335	C14H13Cl4N	060857-30-9	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG090816\
Data File : BG023965.D
Acq On : 8 Sep 2016 12:08
Operator : UM/SJ
Sample : H4680-27
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BH-20-12-15FT

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.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
unknown2.97	2.97	372.7	ng	5083830	1	8.11	272784	20.0
2-Pentanone, 4-hy...	5.18	21.7	ng	295601	1	8.11	272784	20.0
unknown7.64	7.64	129.3	ng	1763000	1	8.11	272784	20.0
Tetradecane	16.46	2.4	ng	113301	4	17.54	939220	20.0
3-Undecene, 8-met...	17.90	3.5	ng	166547	4	17.54	939220	20.0
unknown18.41	18.41	2.9	ng	133787	4	17.54	939220	20.0
Fumaric acid, 2-c...	19.26	11.3	ng	529419	4	17.54	939220	20.0
Decane, 1-iodo-	20.42	2.1	ng	114352	5	21.85	1067660	20.0
2H-Pyran-2-one, t...	20.76	2.4	ng	126948	5	21.85	1067660	20.0
Hexanedioic acid,...	20.88	2.5	ng	131459	5	21.85	1067660	20.0
unknown21.44	21.44	2.6	ng	137012	5	21.85	1067660	20.0