LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF021418\
Data File : BF102980.D
Acq On : 14 Feb 2018 11:06
Operator : SJ/JU
Sample : J1515-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

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_F\METHODS\8270-BF020318.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	2.152	5	11	23	rVB	2346167	3068913	17.44%	5.635%
2	4.475	402	406	413	rBV	317790	345036	1.96%	0.634%
3	5.157	507	522	524	rVB	5619494	17593580	100.00%	32.307%
4	5.492	572	579	583	rBV	1833639	1825015	10.37%	3.351%
5	6.498	746	750	756	rBV	1626554	1381139	7.85%	2.536%
6	6.645	770	775	778	rBV	3191083	3114218	17.70%	5.719%
7	6.875	810	814	817	rBV	1325291	1102512	6.27%	2.025%
8	7.034	836	841	844	rBV	3686067	3549220	20.17%	6.517%
9	7.092	847	851	854	rBV2	245623	188479	1.07%	0.346%
10	7.439	905	910	913	rVB	3051702	3045495	17.31%	5.592%
11	8.157	1024	1032	1038	rBV	1766079	1816283	10.32%	3.335%
12	8.633	1108	1113	1115	rVV3	154742	194354	1.10%	0.357%
13	9.157	1197	1202	1206	rBV2	140271	185369	1.05%	0.340%
14	9.233	1210	1215	1218	rBV	4821390	4917068	27.95%	9.029%
15	9.569	1265	1272	1278	rBV4	85578	183793	1.04%	0.338%
16	9.833	1309	1317	1321	rBV	220902	215471	1.22%	0.396%
17	9.910	1325	1330	1334	rBV	1707416	1675655	9.52%	3.077%
18	10.333	1396	1402	1405	rVB2	219105	219958	1.25%	0.404%
19	10.551	1436	1439	1445	rVB	234992	233144	1.33%	0.428%
20	10.698	1461	1464	1470	rBV	873138	774762	4.40%	1.423%
21	10.804	1479	1482	1488	rBV	138998	183722	1.04%	0.337%
22	11.380	1577	1580	1581	rBV	197590	205349	1.17%	0.377%
23	11.398	1581	1583	1587	rVB	1732113	1556024	8.84%	2.857%
24	12.986	1848	1853	1857	rBV	3913033	4565760	25.95%	8.384%
25	14.039	2028	2032	2039	rVB	1430474	1350130	7.67%	2.479%
26	15.515	2278	2283	2289	rBV	774291	966427	5.49%	1.775%

Sum of corrected areas: 54456876

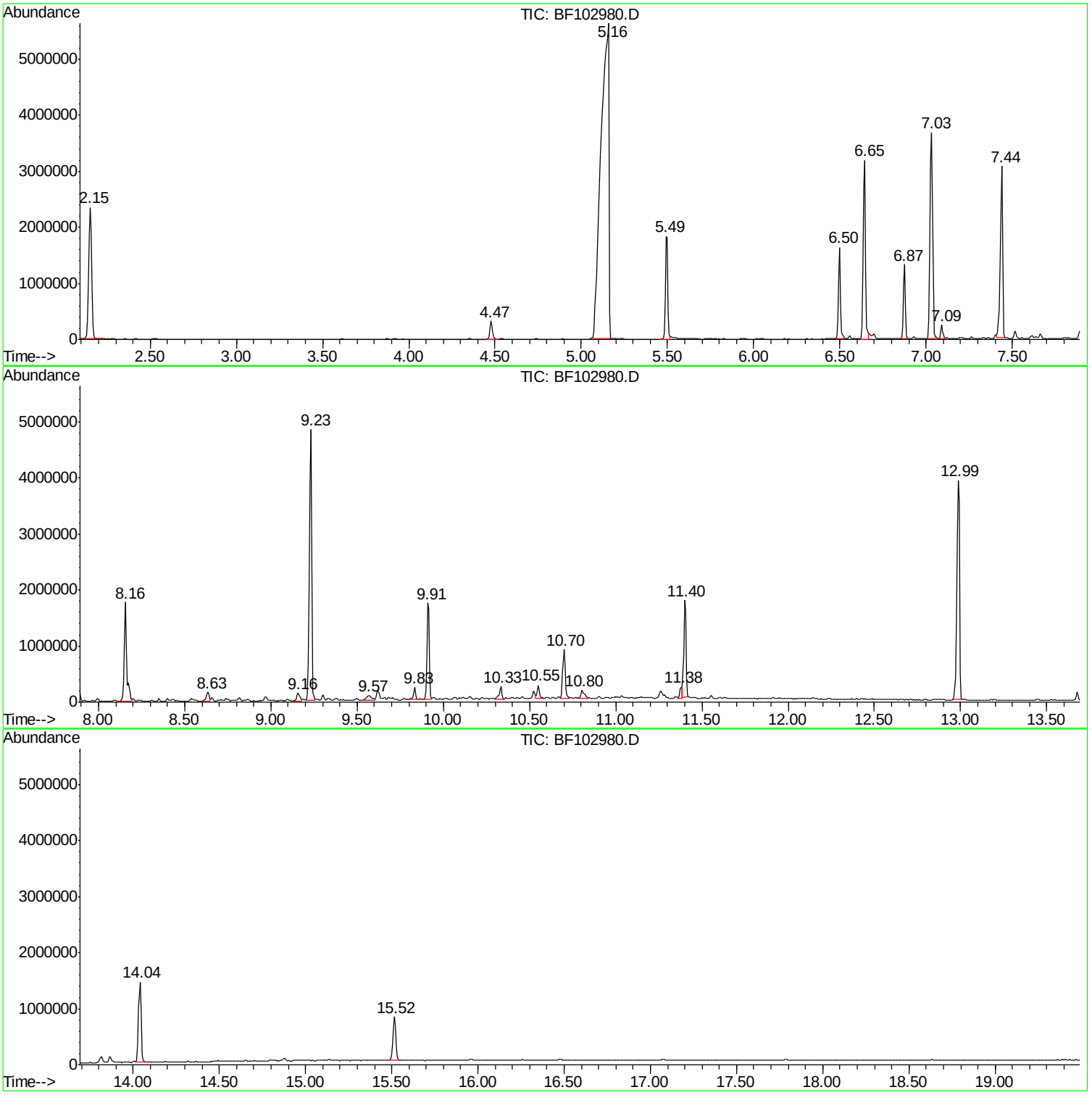
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF021418\
Data File : BF102980.D
Acq On : 14 Feb 2018 11:06
Operator : SJ/JU
Sample : J1515-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF021418\
Data File : BF102980.D
Acq On : 14 Feb 2018 11:06
Operator : SJ/JU
Sample : J1515-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

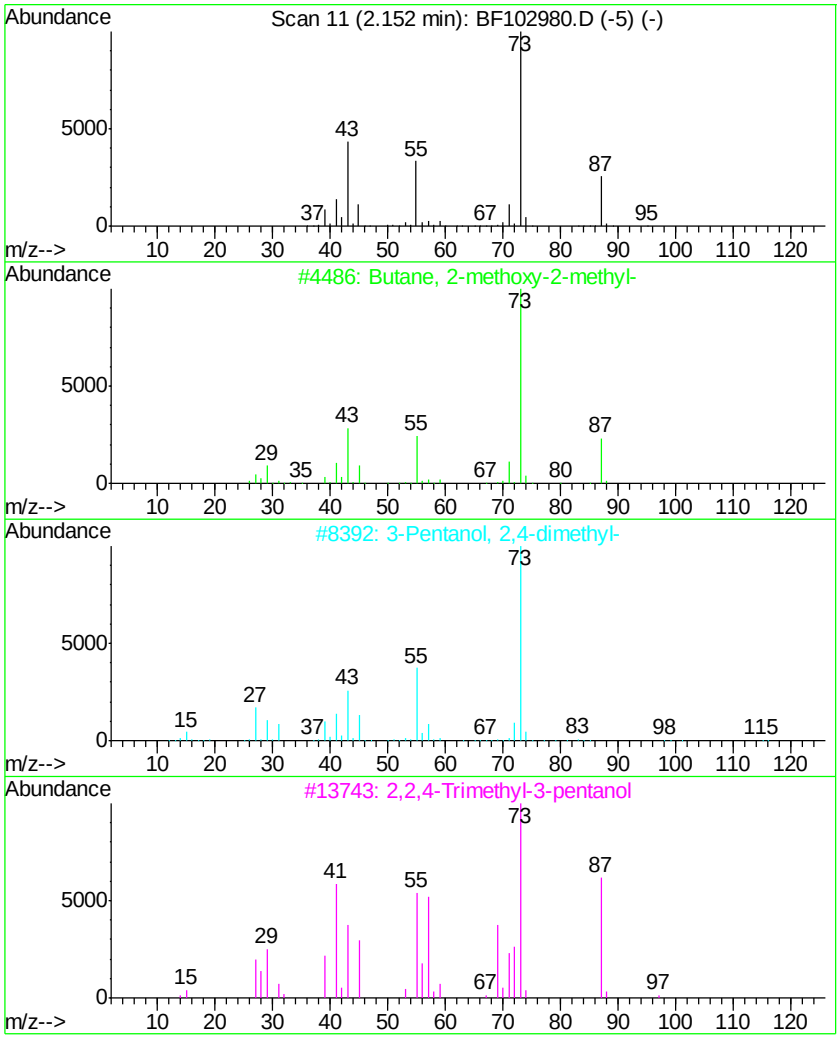
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

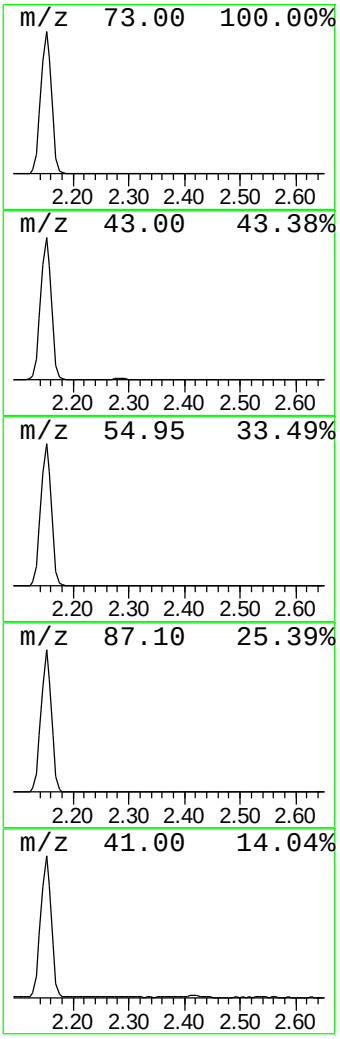
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	55.67 ng	3068910	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\HPCHEM1\BNA F\DATA\BF021418\
Data File : BF102980.D
Acq On : 14 Feb 2018 11:06
Operator : SJ/JU
Sample : J1515-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

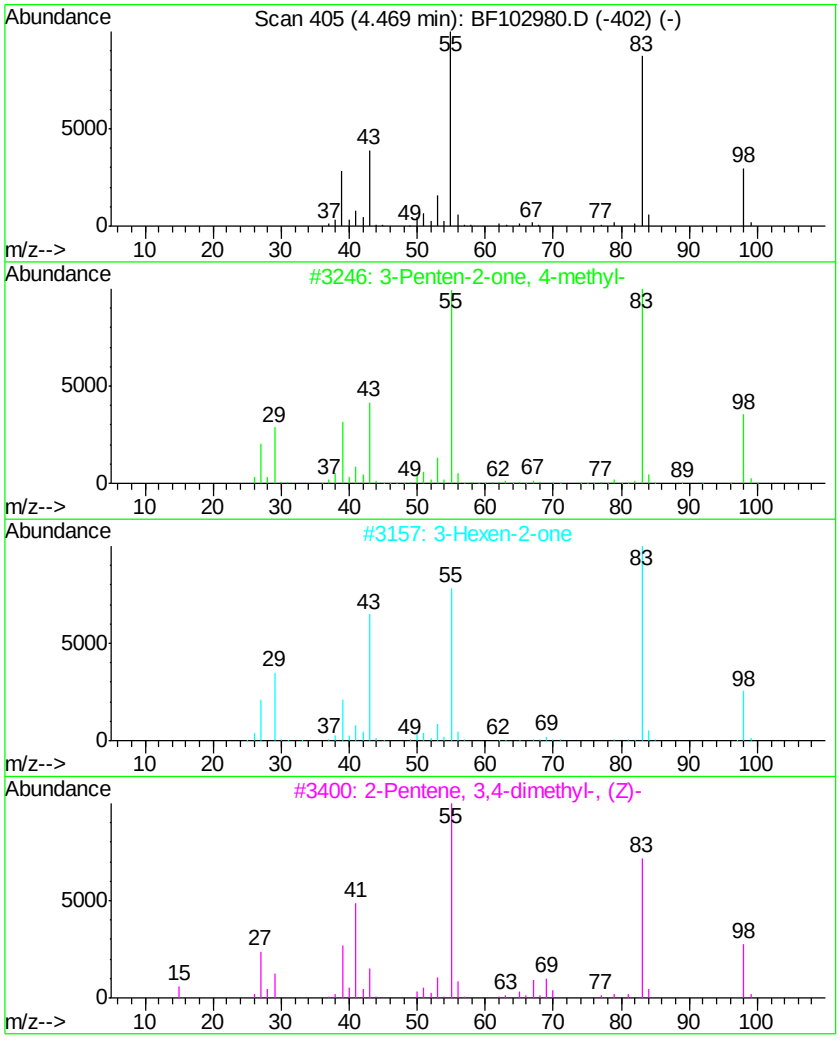
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

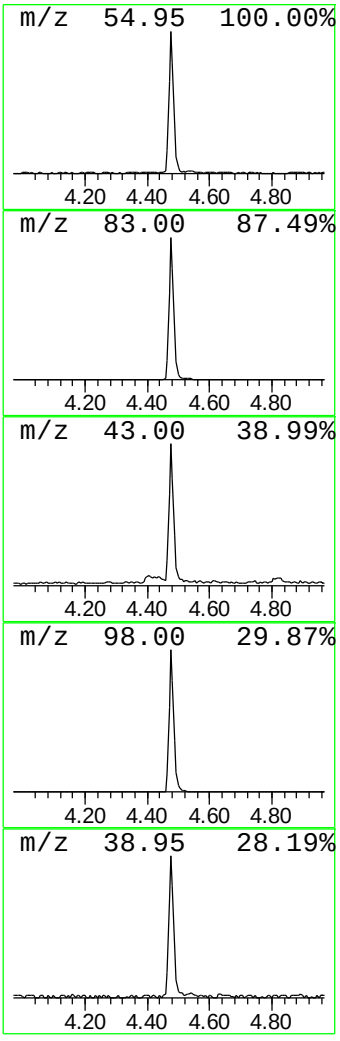
****

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.47	6.26 ng	345036	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF021418\
Data File : BF102980.D
Acq On : 14 Feb 2018 11:06
Operator : SJ/JU
Sample : J1515-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

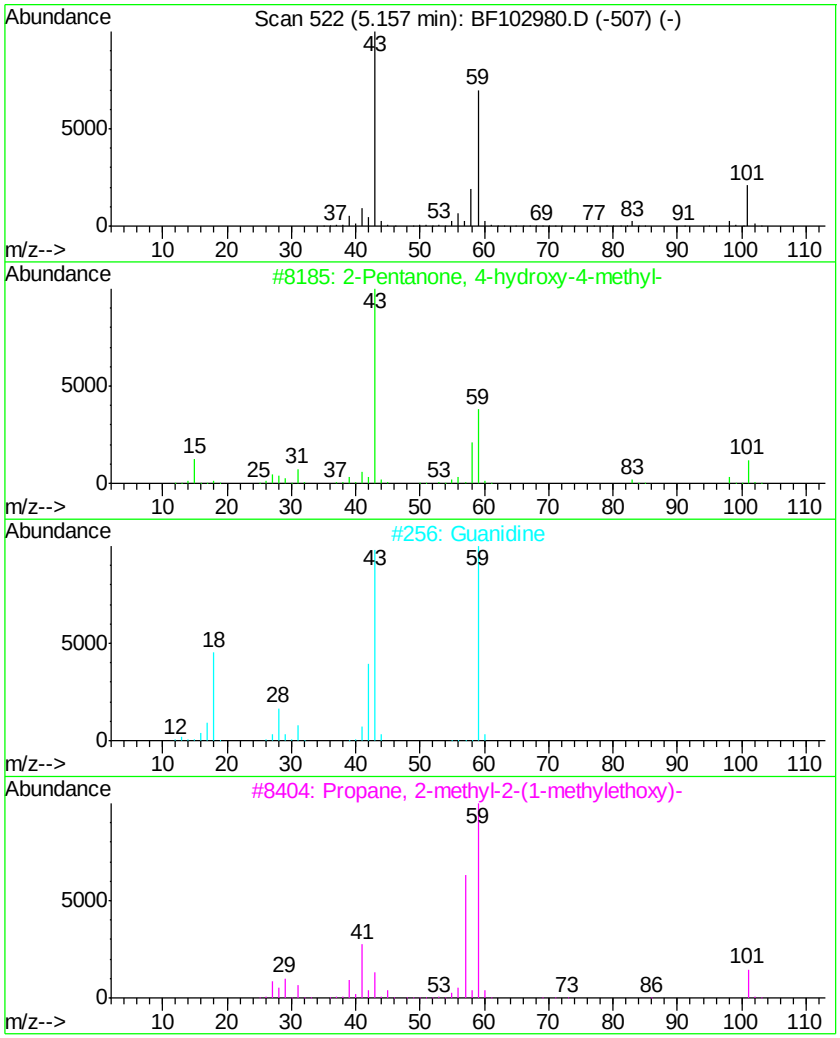
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

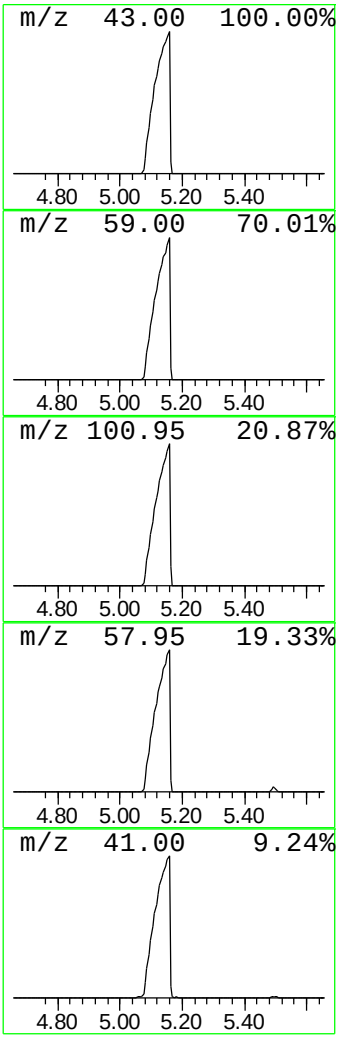
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	319.15 ng	17593600	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Guanidine	59	CH5N3	000113-00-8	38
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF021418\
Data File : BF102980.D
Acq On : 14 Feb 2018 11:06
Operator : SJ/JU
Sample : J1515-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

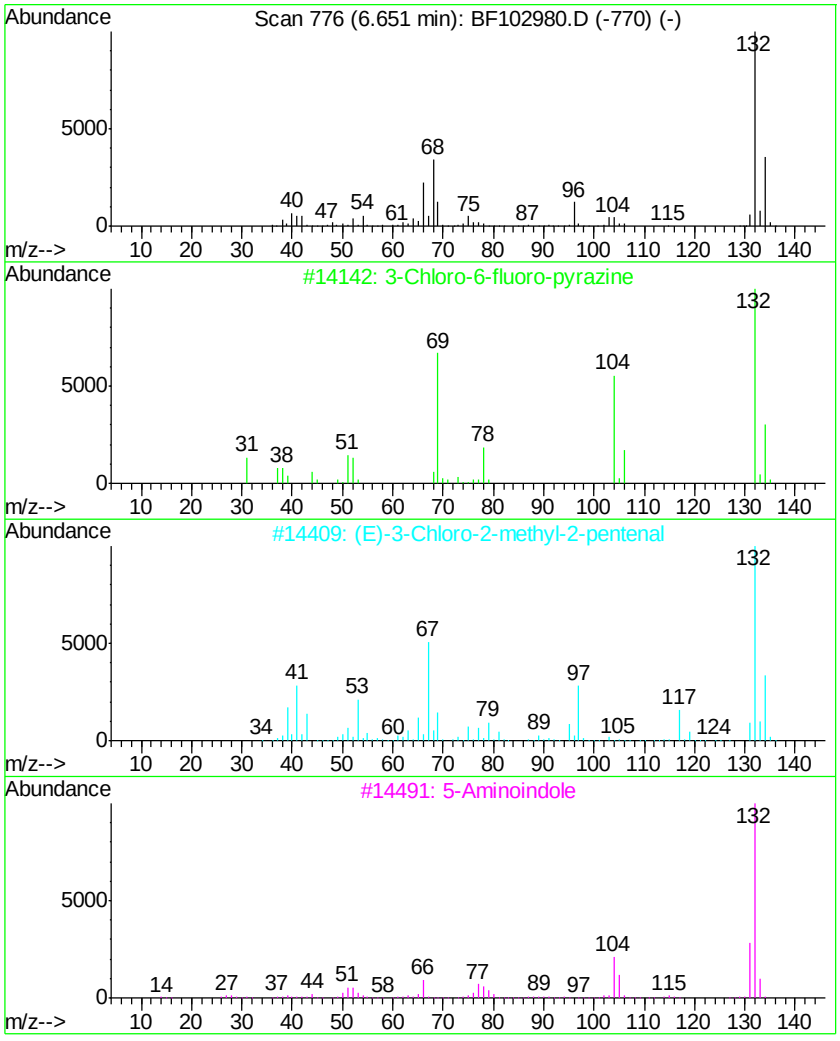
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

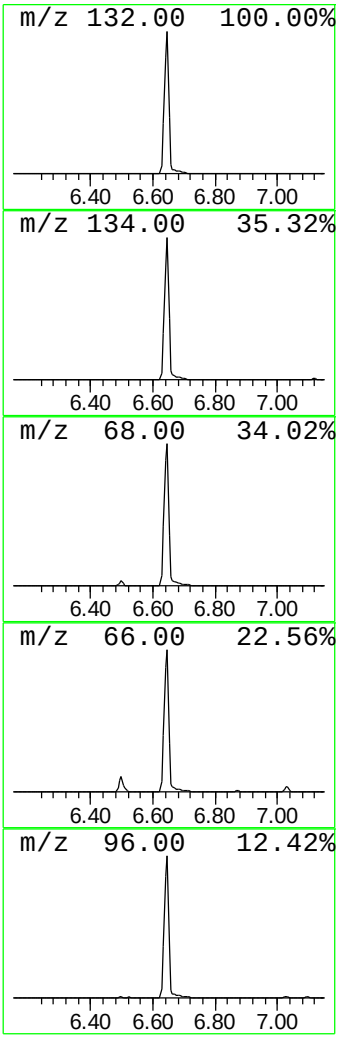
****

Peak Number 4 unknown6.65 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	56.49 ng	3114220	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF021418\
Data File : BF102980.D
Acq On : 14 Feb 2018 11:06
Operator : SJ/JU
Sample : J1515-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

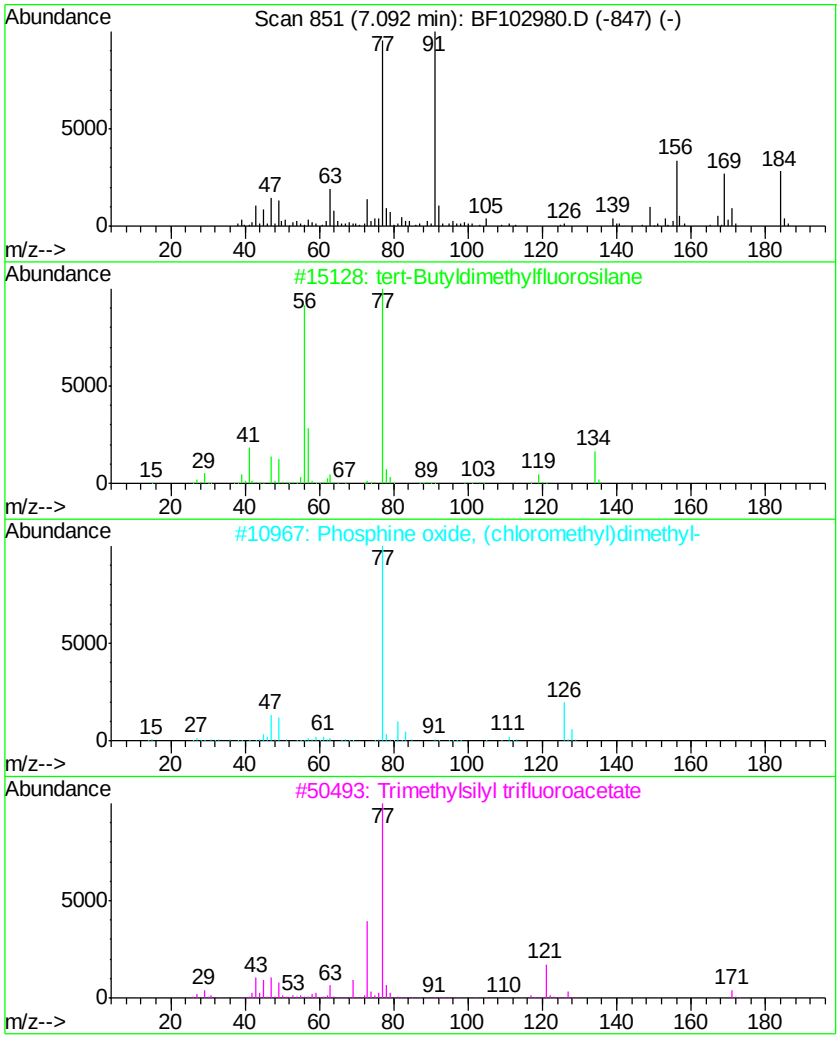
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

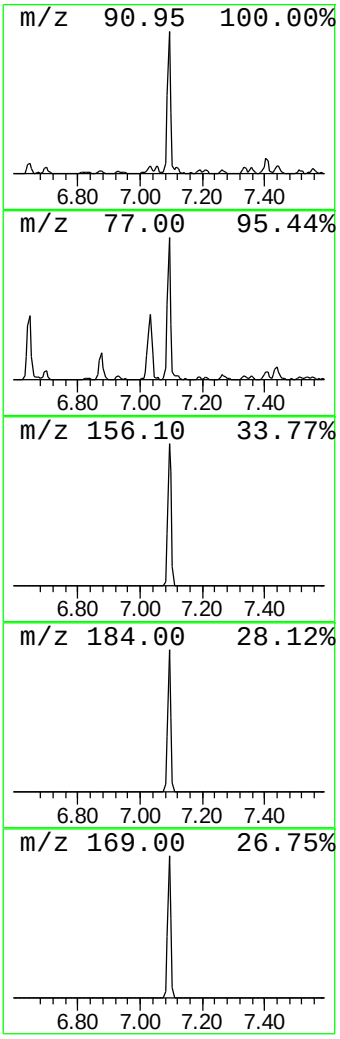
****

Peak Number 6 unknown7.09 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.09	3.42 ng	188479	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	tert-Butyldimethylfluorosilane	134	C6H15FSi	1000366-62-3	38
2	Phosphine oxide, (chloromethyl)d...	126	C3H8ClOP	001638-75-1	38
3	Trimethylsilyl trifluoroacetate	186	C5H9F3O2Si	000400-53-3	32
4	3-Methyl-7-phenylhepta-1,3,4-triene	184	C14H16	103240-61-5	30
5	1-Triazene, 3,3-dimethyl-1-phenyl-	149	C8H11N3	007227-91-0	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF021418\
Data File : BF102980.D
Acq On : 14 Feb 2018 11:06
Operator : SJ/JU
Sample : J1515-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

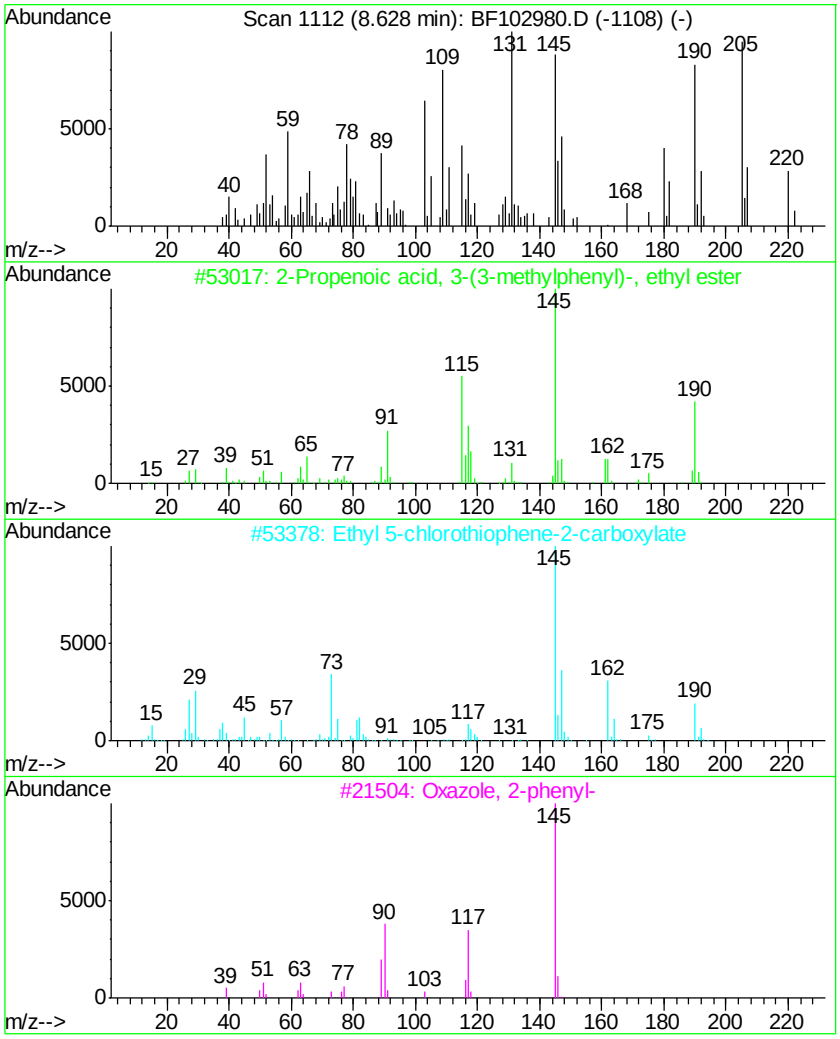
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

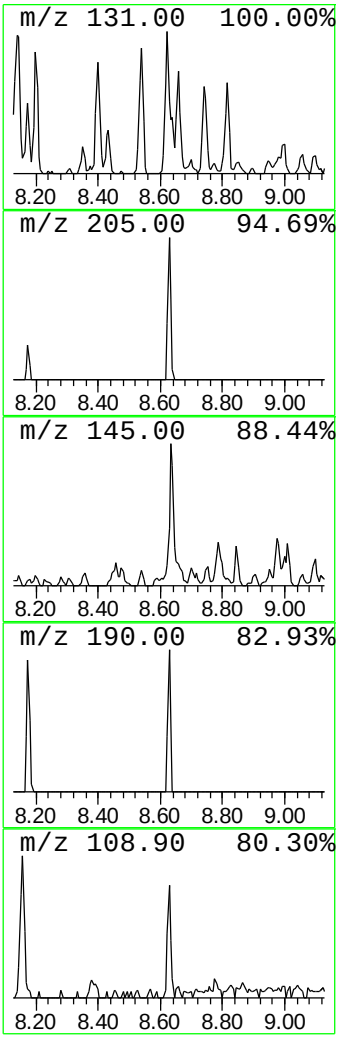
****

Peak Number 7 unknown8.63 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.63	2.14 ng	194354	Naphthalene-d8	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenoic acid, 3-(3-methylphe...	190	C12H14O2	050556-03-1	22
2	Ethyl 5-chlorothiophene-2-carbox...	190	C7H7ClO2S	005751-82-6	18
3	Oxazole, 2-phenyl-	145	C9H7NO	020662-88-8	18
4	Benzene, (1,3-dimethyl-2-butenyl)-	160	C12H16	050704-01-3	14
5	2-Chloro-4-fluoroaniline	145	C6H5ClFN	002106-02-7	14





Data Path : Z:\HPCHEM1\BNA F\DATA\BF021418\
Data File : BF102980.D
Acq On : 14 Feb 2018 11:06
Operator : SJ/JU
Sample : J1515-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

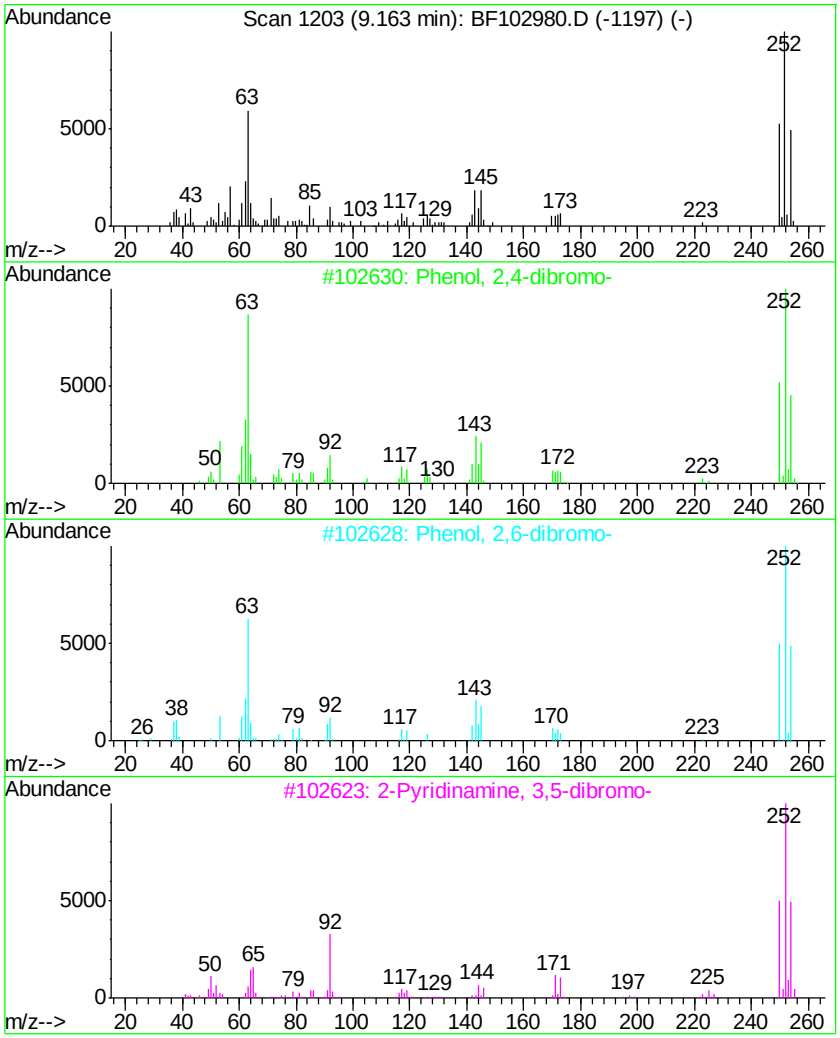
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

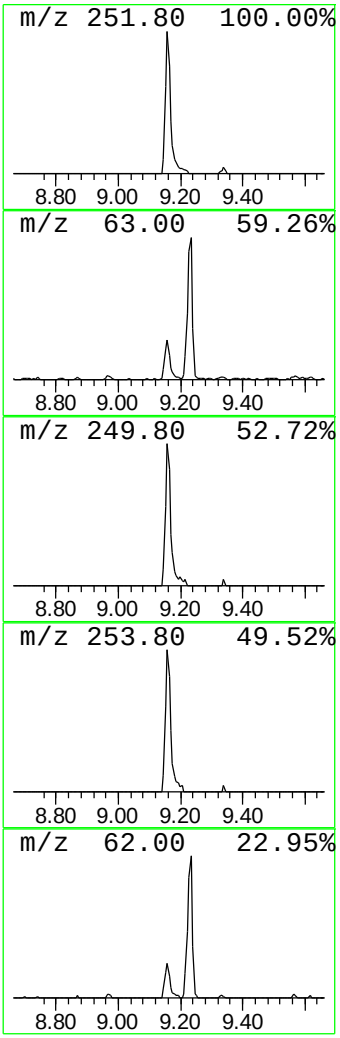
****

Peak Number 8 Phenol, 2,4-dibromo- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.16	2.21 ng	185369	Acenaphthene-d10	9.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,4-dibromo-	250	C6H4Br2O	000615-58-7	99
2	Phenol, 2,6-dibromo-	250	C6H4Br2O	000608-33-3	98
3	2-Pyridinamine, 3,5-dibromo-	250	C5H4Br2N2	035486-42-1	50
4	2-Chloroethyl carbonate	186	C5H8Cl2O3	000623-97-2	38
5	Propanoic acid, 2-chloro-, ethyl...	136	C5H9ClO2	000535-13-7	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF021418\
Data File : BF102980.D
Acq On : 14 Feb 2018 11:06
Operator : SJ/JU
Sample : J1515-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

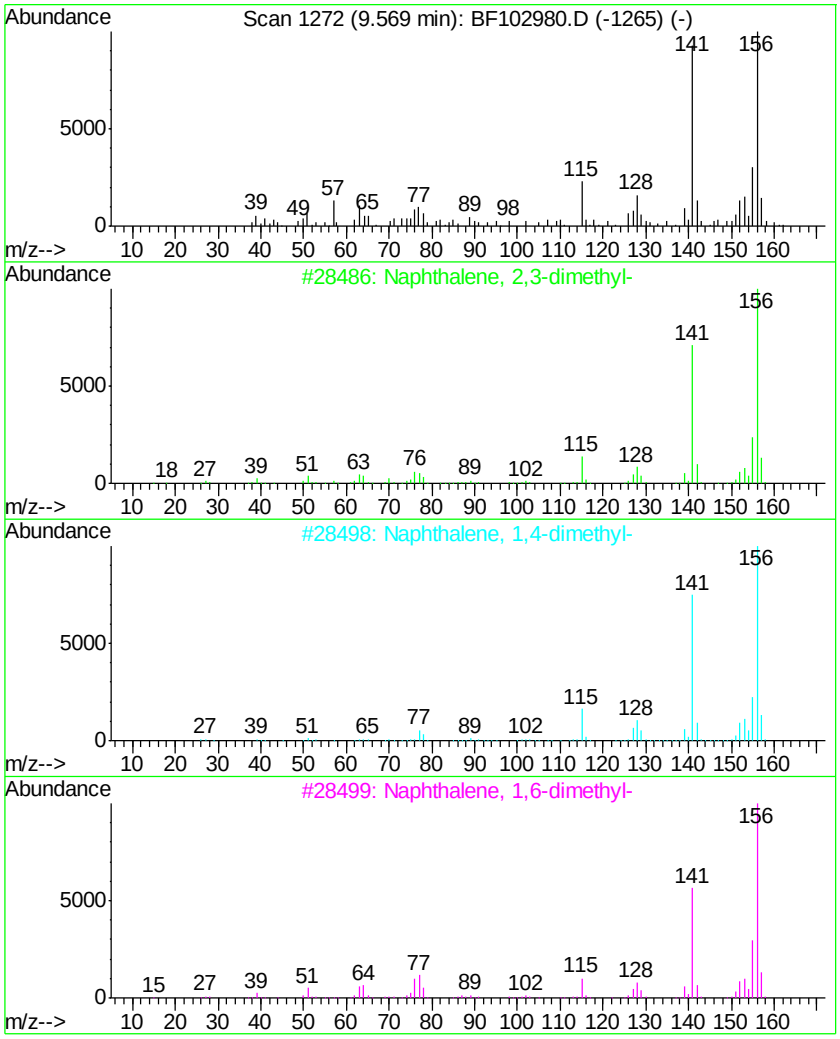
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

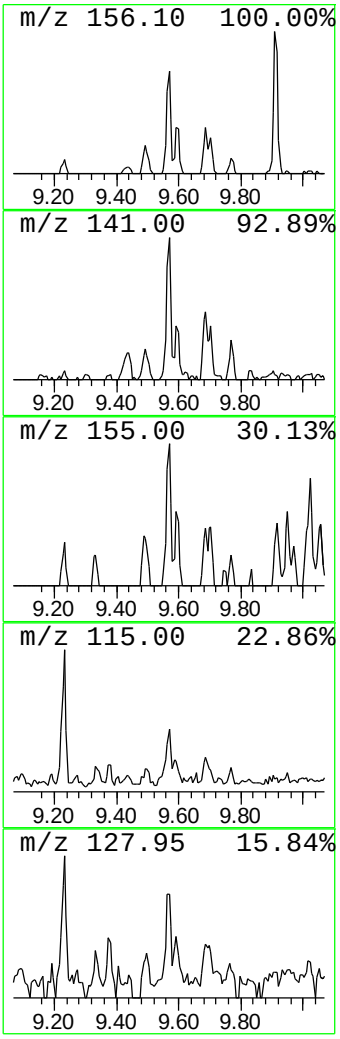
****

Peak Number 9 Naphthalene, 2,3-dimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.57	2.19 ng	183793	Acenaphthene-d10	9.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
2	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
3	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
4	Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	96
5	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	96





Data Path : Z:\HPCHEM1\BNA F\DATA\BF021418\
Data File : BF102980.D
Acq On : 14 Feb 2018 11:06
Operator : SJ/JU
Sample : J1515-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

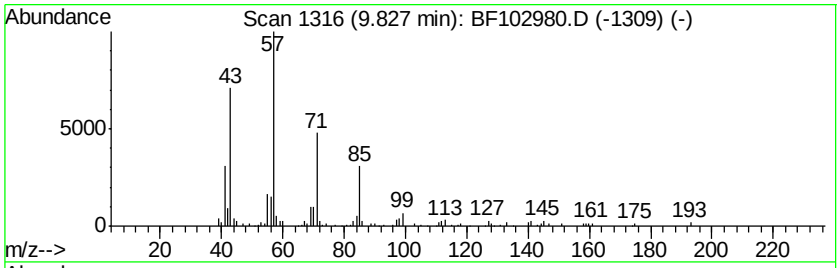
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

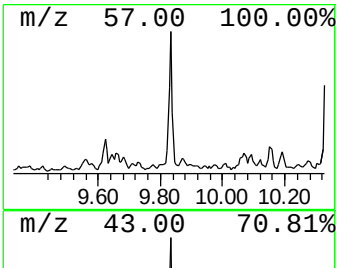
****

Peak Number 10 Tetradecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.83	2.57 ng	215471	Acenaphthene-d10	9.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	90
2	Hexadecane	226	C16H34	000544-76-3	87
3	Tridecane	184	C13H28	000629-50-5	86
4	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	80
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	78





Data Path : Z:\HPCHEM1\BNA F\DATA\BF021418\
Data File : BF102980.D
Acq On : 14 Feb 2018 11:06
Operator : SJ/JU
Sample : J1515-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

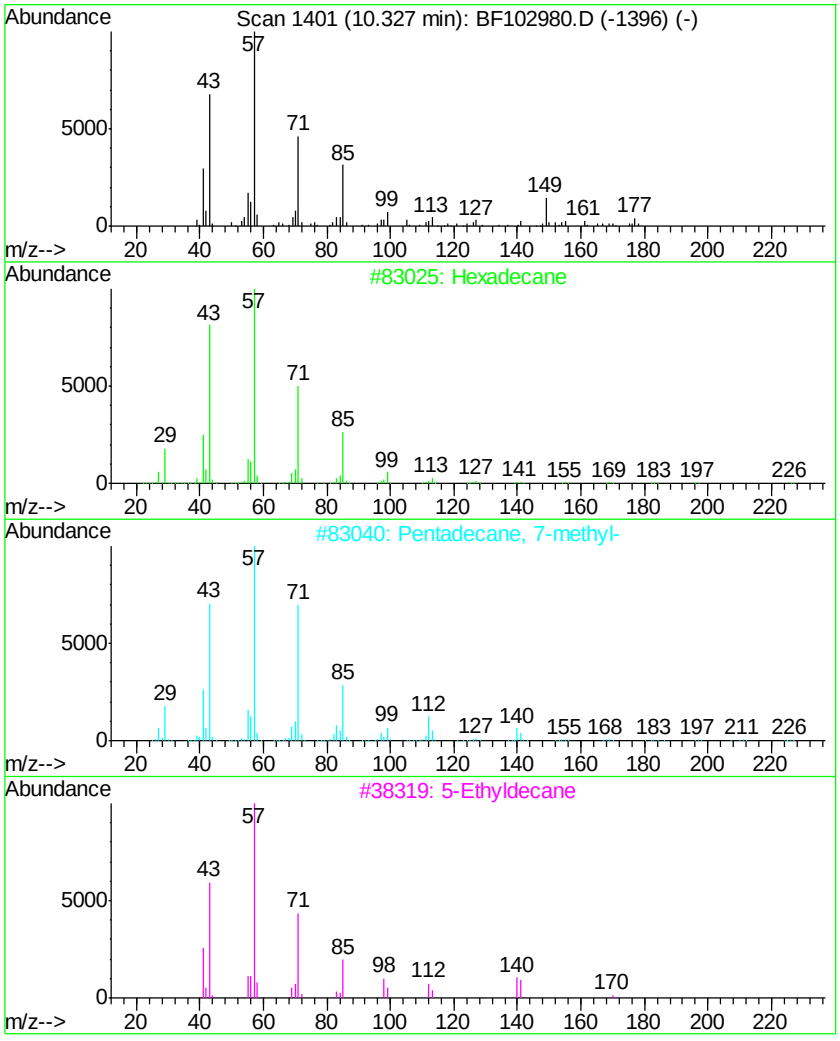
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

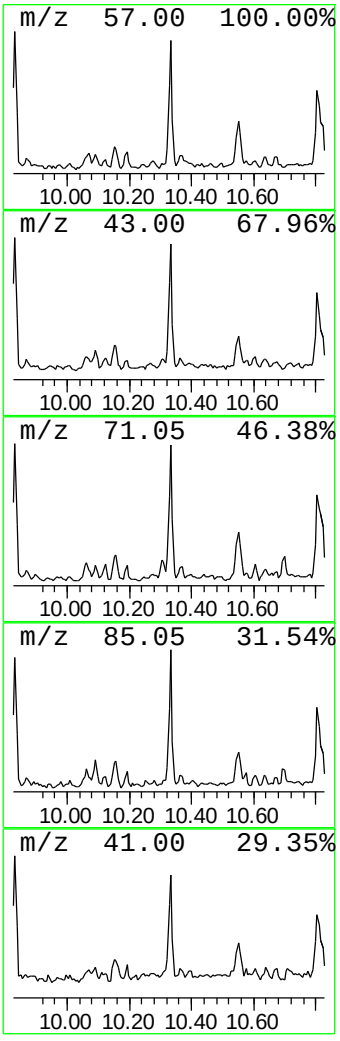
****

Peak Number 11 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.33	2.63 ng	219958	Acenaphthene-d10	9.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	93
2	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	90
3	5-Ethyldecane	170	C12H26	017302-36-2	90
4	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86
5	Tridecane	184	C13H28	000629-50-5	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF021418\
Data File : BF102980.D
Acq On : 14 Feb 2018 11:06
Operator : SJ/JU
Sample : J1515-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

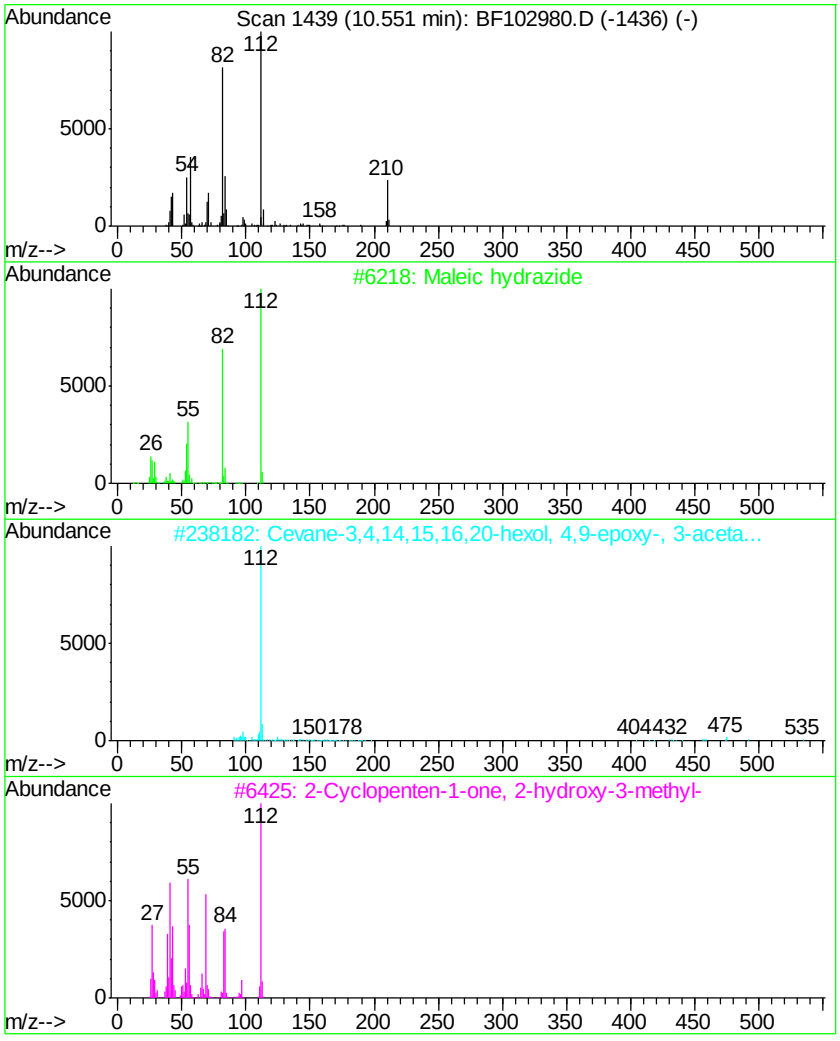
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

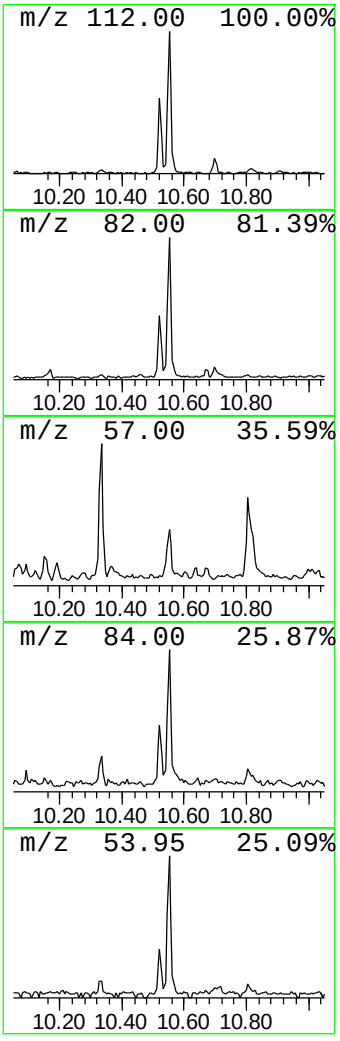
****

Peak Number 12 Maleic hydrazide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.55	2.78 ng	233144	Acenaphthene-d10	9.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Maleic hydrazide	112	C4H4N2O2	000123-33-1	59
2	Cevane-3,4,14,15,16,20-hexol, 4,...	535	C29H45NO8	002777-79-9	50
3	2-Cyclopenten-1-one, 2-hydroxy-3...	112	C6H8O2	000080-71-7	35
4	Phenol, 4-fluoro-	112	C6H5FO	000371-41-5	35
5	5-Azacytosine	112	C3H4N4O	000931-86-2	30





Data Path : Z:\HPCHEM1\BNA F\DATA\BF021418\
Data File : BF102980.D
Acq On : 14 Feb 2018 11:06
Operator : SJ/JU
Sample : J1515-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

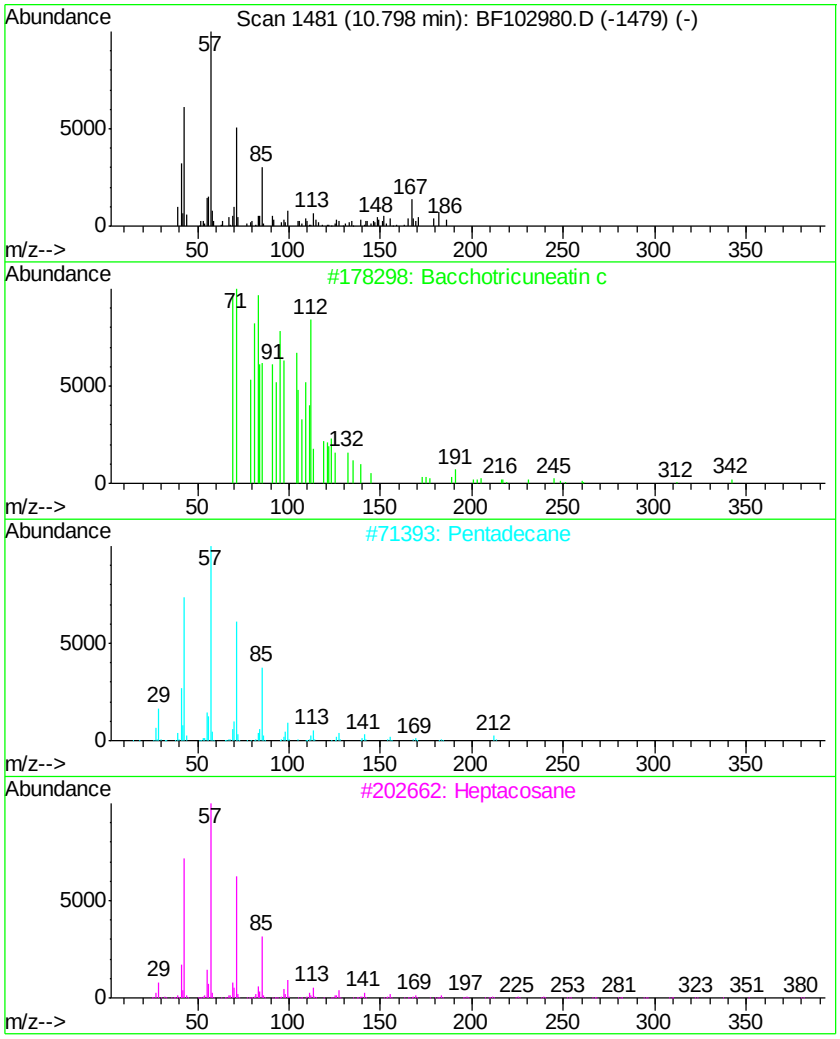
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

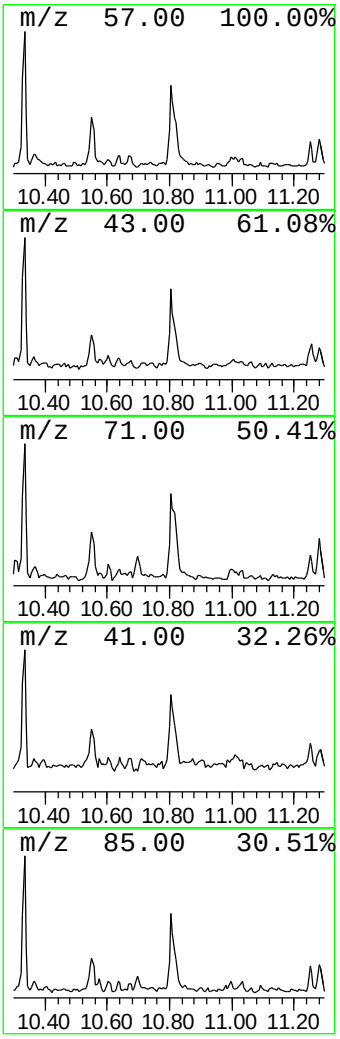
****

Peak Number 13 Bacchotricuneatin c Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	2.36 ng	183722	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bacchotricuneatin c	342	C20H22O5	066563-30-2	91
2	Pentadecane	212	C15H32	000629-62-9	86
3	Heptacosane	380	C27H56	000593-49-7	86
4	Hexadecane	226	C16H34	000544-76-3	86
5	Eicosane	282	C20H42	000112-95-8	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021418\
Data File : BF102980.D
Acq On : 14 Feb 2018 11:06
Operator : SJ/JU
Sample : J1515-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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
Butane, 2-methoxy...	2.15	55.7	ng	3068910	1	6.87	1102510	20.0
3-Penten-2-one, 4...	4.47	6.3	ng	345036	1	6.87	1102510	20.0
2-Pentanone, 4-hy...	5.16	319.1	ng	17593600	1	6.87	1102510	20.0
unknown6.65	6.65	56.5	ng	3114220	1	6.87	1102510	20.0
unknown7.09	7.09	3.4	ng	188479	1	6.87	1102510	20.0
unknown8.63	8.63	2.1	ng	194354	2	8.16	1816280	20.0
Phenol, 2,4-dibromo-	9.16	2.2	ng	185369	3	9.91	1675660	20.0
Naphthalene, 2,3-...	9.57	2.2	ng	183793	3	9.91	1675660	20.0
Tetradecane	9.83	2.6	ng	215471	3	9.91	1675660	20.0
Hexadecane	10.33	2.6	ng	219958	3	9.91	1675660	20.0
Maleic hydrazide	10.55	2.8	ng	233144	3	9.91	1675660	20.0
Bacchotricuneatin c	10.80	2.4	ng	183722	4	11.40	1556020	20.0