LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080218\
Data File : BF107925.D
Acq On : 2 Aug 2018 22:28
Operator : JU/SJ
Sample : J4285-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KG-PIT-3

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_F\METHODS\8270-BF073018.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	5.184	480	484	502	rBV	210399	334125	14.08%	1.855%
2	5.595	551	554	580	rBV	674251	1790490	75.44%	9.939%
3	6.601	721	725	743	rBV	749933	1882938	79.33%	10.452%
4	6.731	743	747	772	rVB	1359789	2373410	100.00%	13.174%
5	6.954	781	785	805	rBV	313051	692969	29.20%	3.846%
6	7.107	807	811	834	rBV	1320500	1706024	71.88%	9.470%
7	7.525	878	882	904	rBV	520950	1318923	55.57%	7.321%
8	8.236	999	1003	1027	rBV	529686	1001617	42.20%	5.560%
9	8.801	1096	1099	1103	rBV	54470	43716	1.84%	0.243%
10	8.954	1121	1125	1129	rBV	36774	60638	2.55%	0.337%
11	9.048	1136	1141	1152	rBV4	65106	164765	6.94%	0.915%
12	9.307	1181	1185	1193	rBV	1603103	1924198	81.07%	10.681%
13	9.366	1193	1195	1199	rVB	91658	96198	4.05%	0.534%
14	9.701	1246	1252	1258	rVB	195803	260868	10.99%	1.448%
15	9.860	1275	1279	1283	rBV2	48765	72253	3.04%	0.401%
16	9.895	1283	1285	1289	rVB	122372	108411	4.57%	0.602%
17	9.989	1298	1301	1313	rVB	611483	747445	31.49%	4.149%
18	10.395	1365	1370	1374	rBV	185001	206903	8.72%	1.148%
19	10.619	1404	1408	1410	rBV	82098	87650	3.69%	0.487%
20	10.789	1433	1437	1448	rBV	691189	1135356	47.84%	6.302%
21	10.872	1448	1451	1456	rVV	270590	373445	15.73%	2.073%
22	11.325	1525	1528	1530	rBV	292645	264737	11.15%	1.469%
23	11.495	1553	1557	1559	rBV	445297	587719	24.76%	3.262%
24	13.083	1825	1827	1833	rVB	805351	780785	32.90%	4.334%

Sum of corrected areas: 18015583

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080218\
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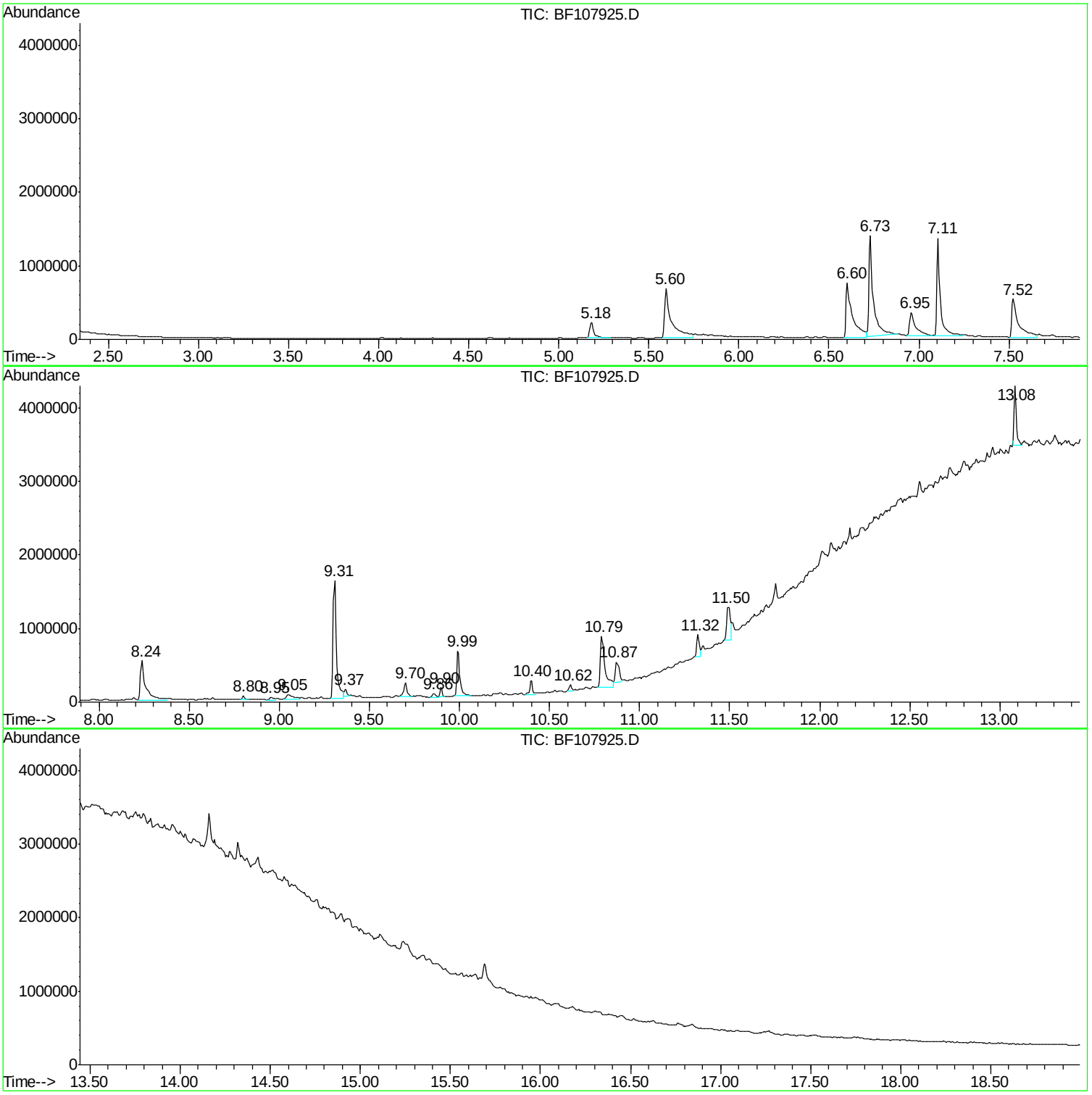
Operator : JU/SJ
Sample : J4285-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KG-PIT-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.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

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Operator : JU/SJ
Sample : J4285-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KG-PIT-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

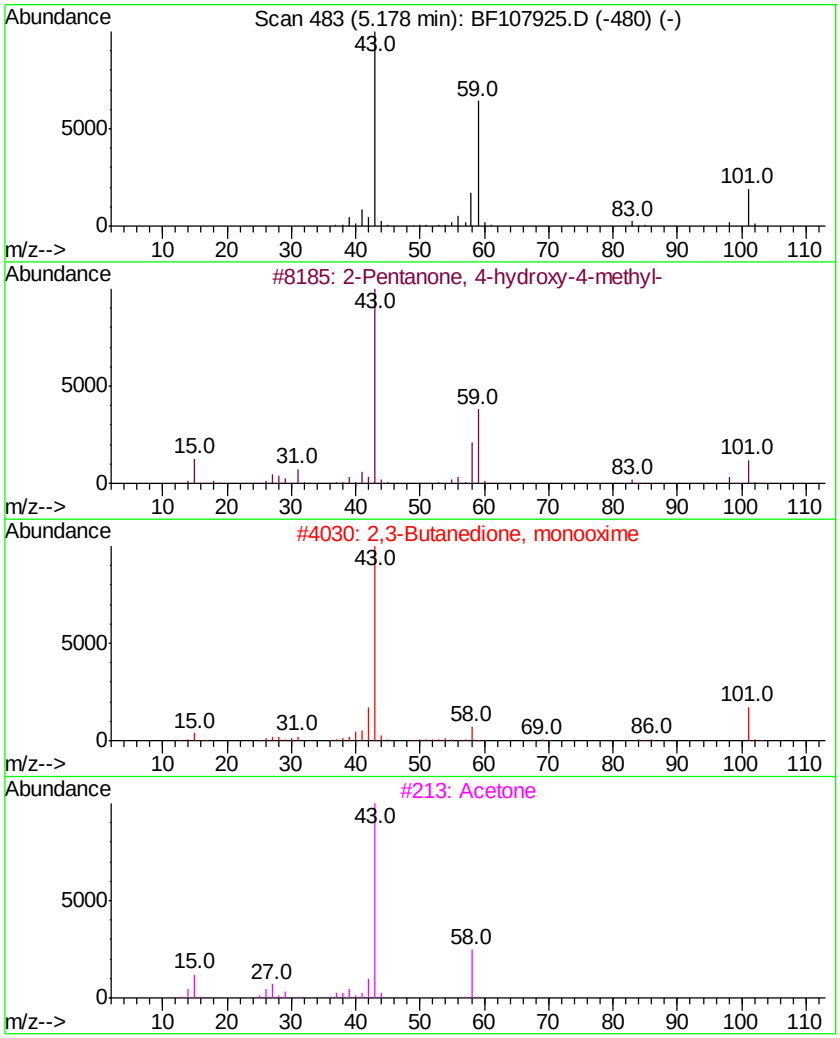
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

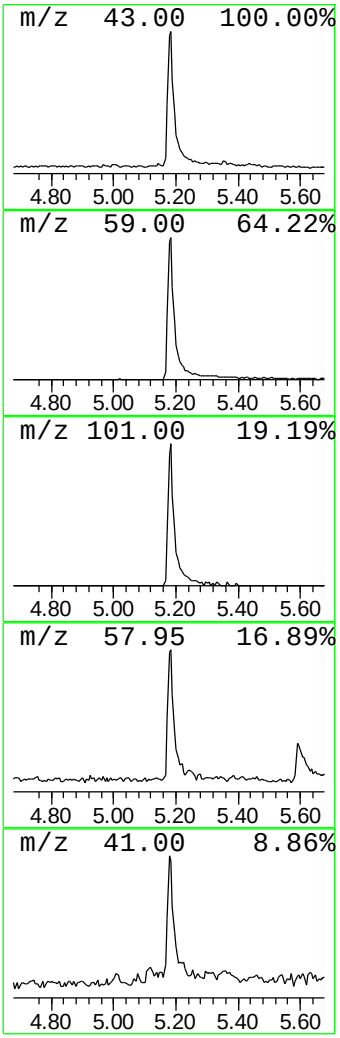
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	9.64 ng	334125	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3	Acetone	58	C3H6O	000067-64-1	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Guanidine	59	CH5N3	000113-00-8	9





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Operator : JU/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : KG-PIT-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
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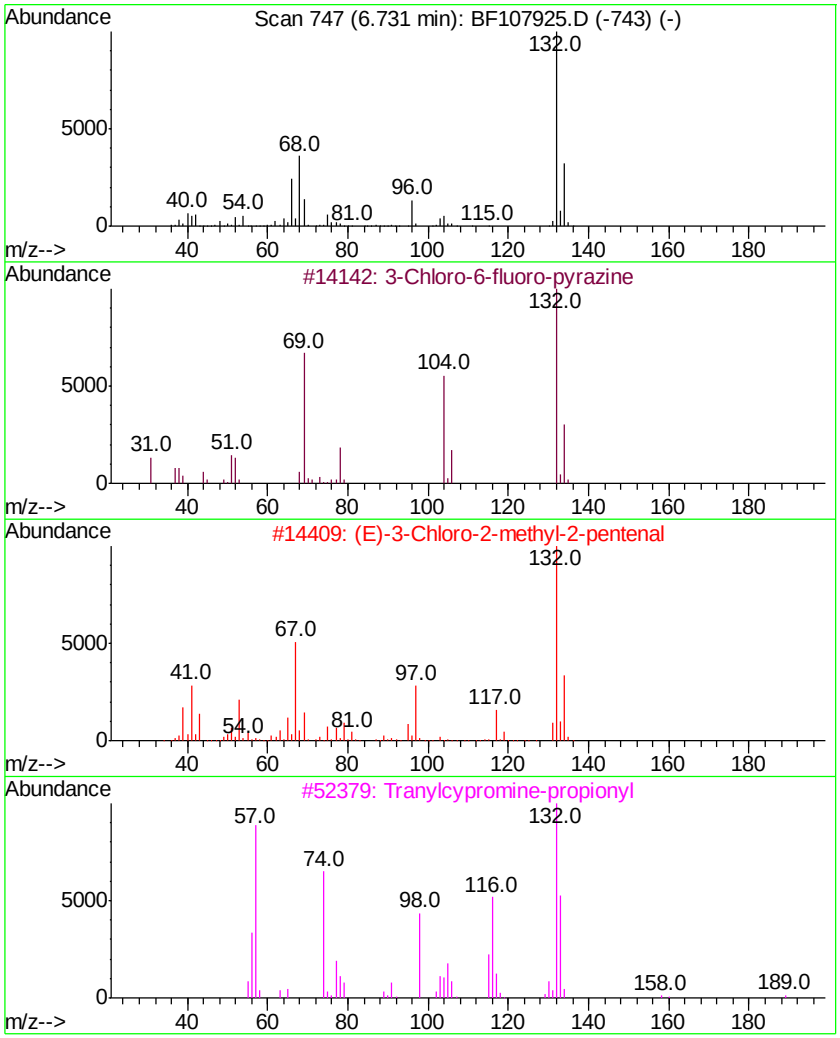
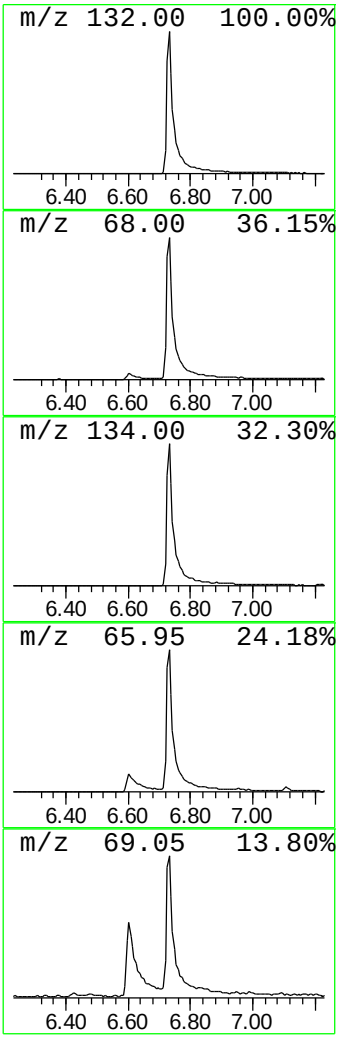
****

Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	68.50 ng	2373410	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

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Data File : BF107925.D
Acq On : 2 Aug 2018 22:28
Operator : JU/SJ
Sample : J4285-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KG-PIT-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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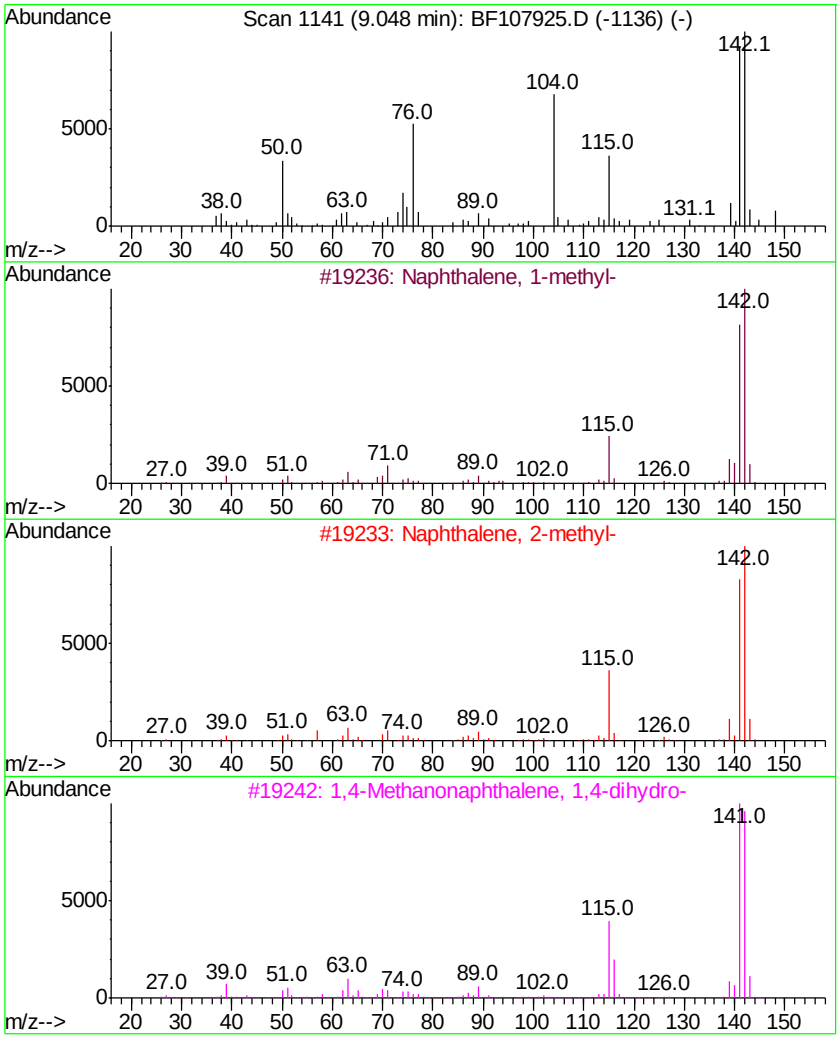
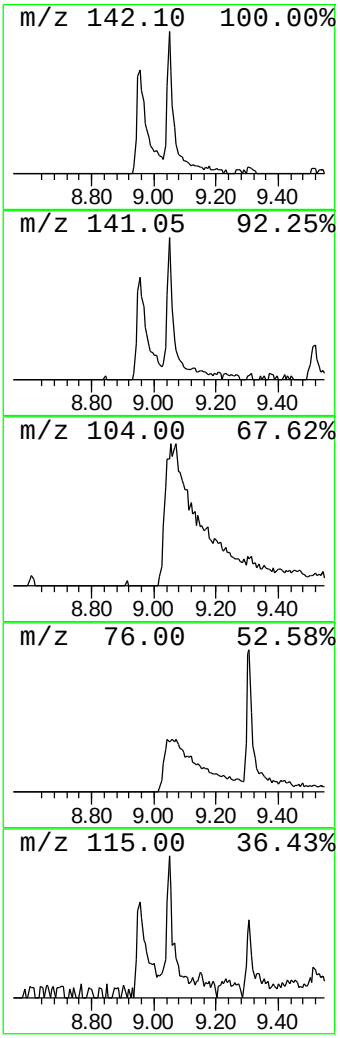
Peak Number 4 Naphthalene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.05	3.29 ng	164765	Naphthalene-d8	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	64
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	60
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	60
4	Benzocycloheptatriene	142	C11H10	000264-09-5	58
5	3,4-Difluorobenzaldehyde	142	C7H4F2O	034036-07-2	46





Library Search Compound Report

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Acq On : 2 Aug 2018 22:28
Operator : JU/SJ
Sample : J4285-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KG-PIT-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.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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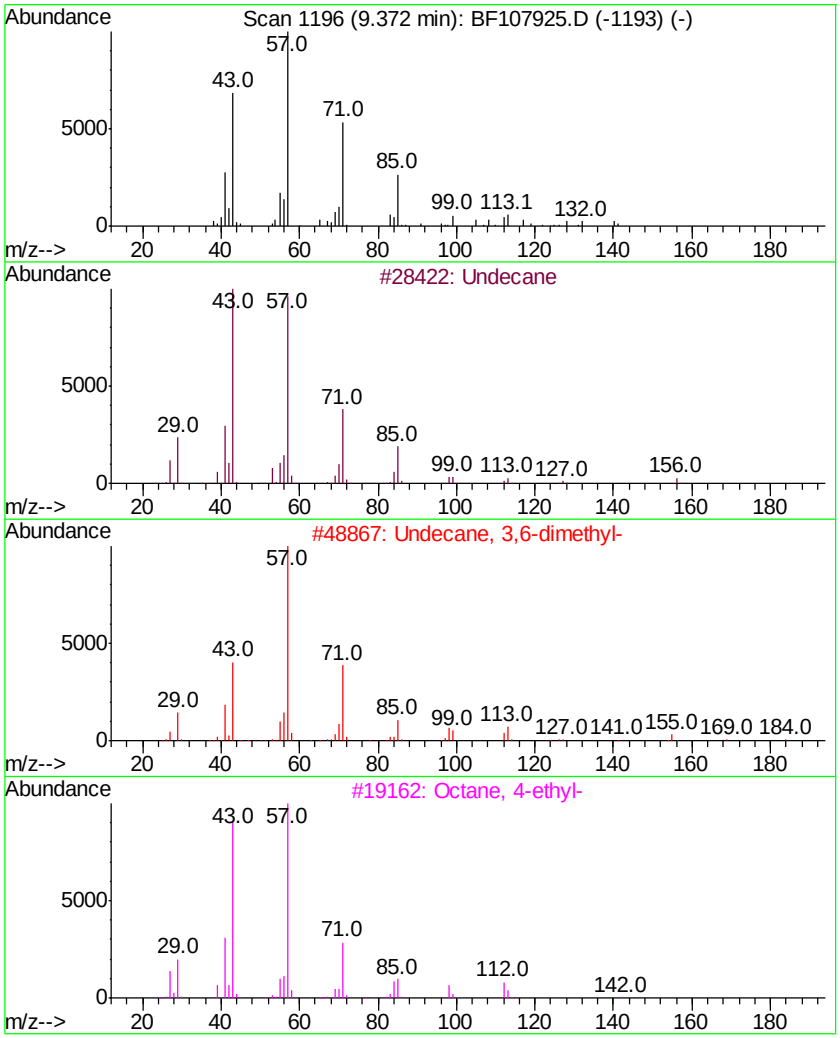
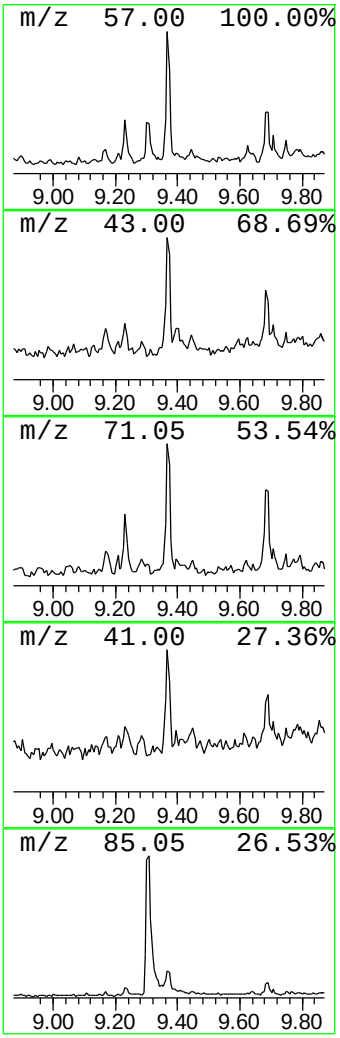
Peak Number 5 Undecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.37	2.57 ng	96198	Acenaphthene-d10	9.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	72
2	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	64
3	Octane, 4-ethyl-	142	C10H22	015869-86-0	64
4	Undecane, 5-methyl-	170	C12H26	001632-70-8	64
5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	59





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080218\
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Operator : JU/SJ
Sample : J4285-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KG-PIT-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

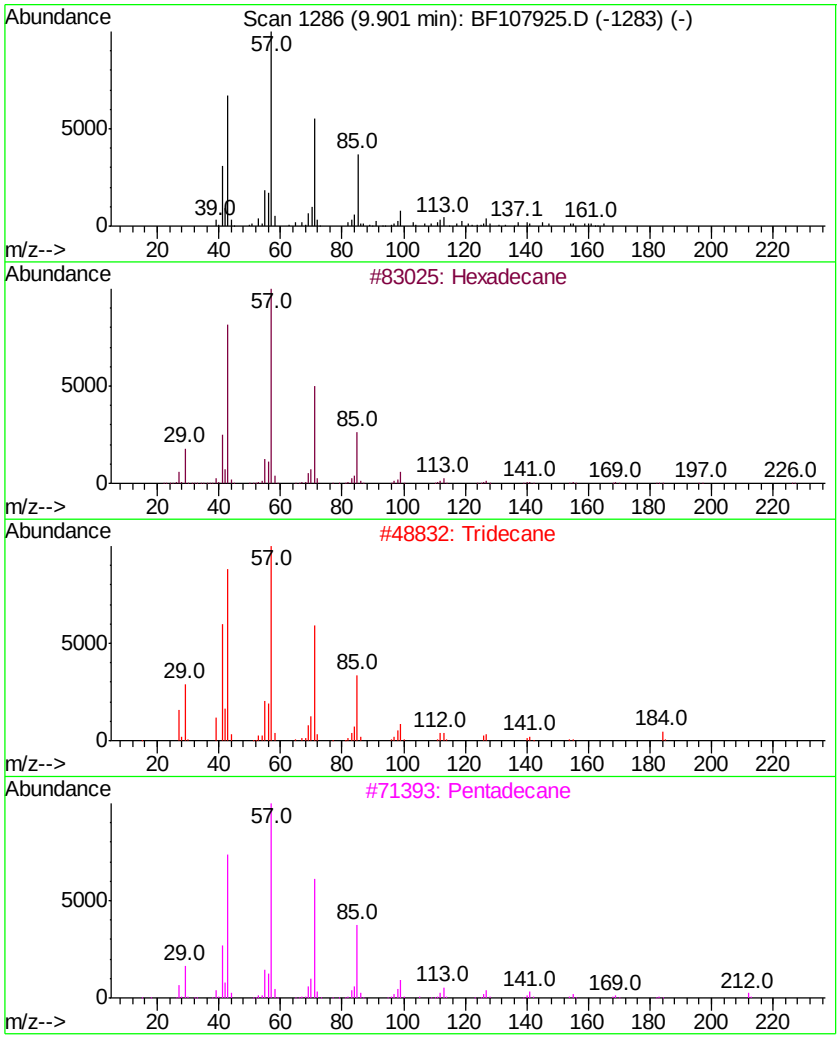
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

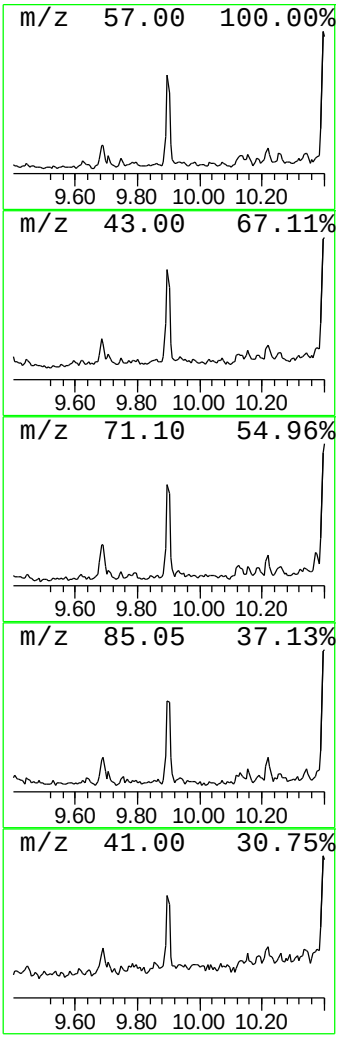
****

Peak Number 6 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.90	2.90 ng	108411	Acenaphthene-d10	9.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Tridecane	184	C13H28	000629-50-5	90
3	Pentadecane	212	C15H32	000629-62-9	90
4	Tetradecane	198	C14H30	000629-59-4	80
5	Tridecane, 6-methyl-	198	C14H30	013287-21-3	78





Library Search Compound Report

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Acq On : 2 Aug 2018 22:28
Operator : JU/SJ
Sample : J4285-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KG-PIT-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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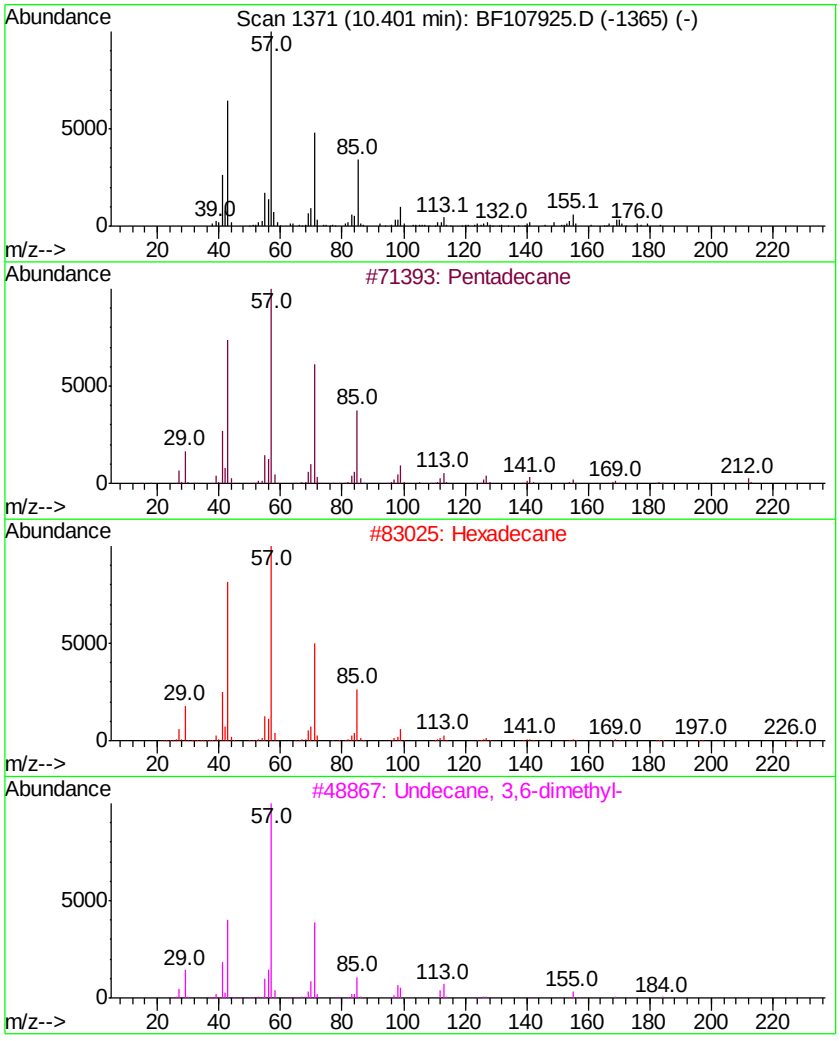
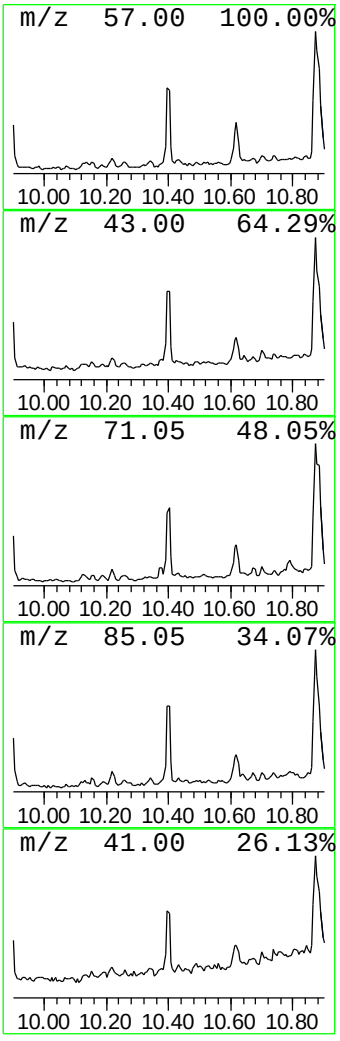
****

Peak Number 7 Pentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.40	5.54 ng	206903	Acenaphthene-d10	9.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	72
2	Hexadecane	226	C16H34	000544-76-3	72
3	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	64
4	Dodecane	170	C12H26	000112-40-3	64
5	Undecane	156	C11H24	001120-21-4	64





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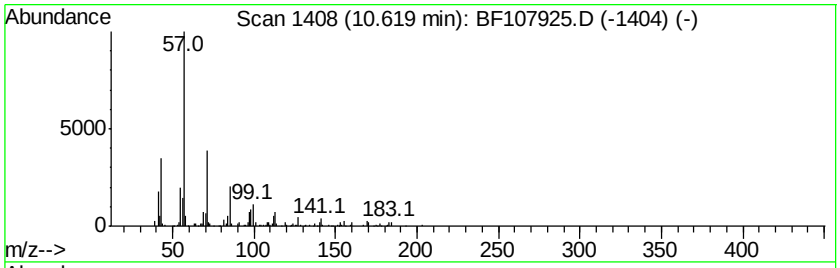
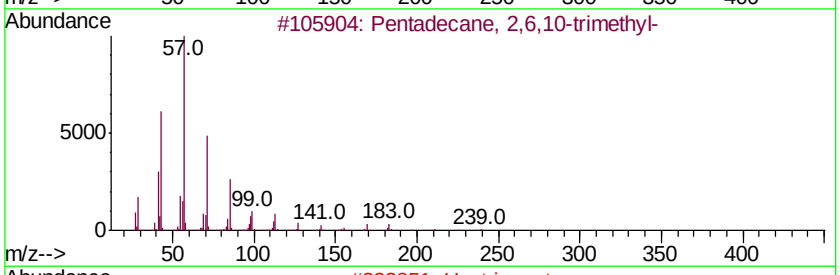
****

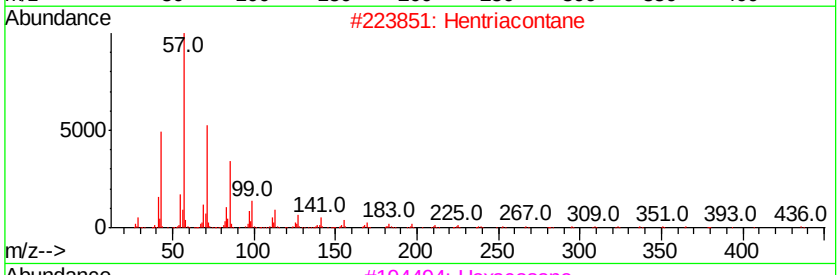
Peak Number 8 Pentadecane, 2,6,10-trimethyl- Concentration Rank 10

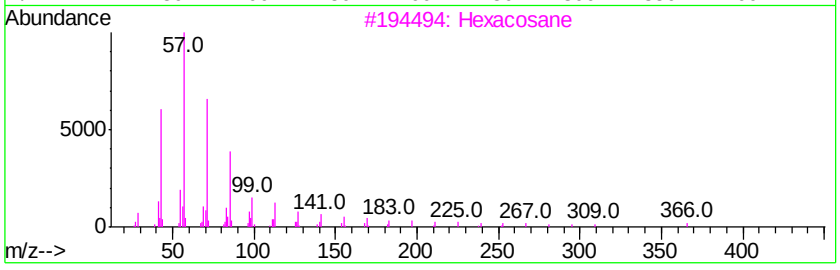
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.62	2.35 ng	87650	Acenaphthene-d10	9.99

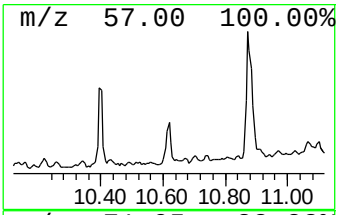
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	86
2	Hentriacontane	437	C31H64	000630-04-6	80
3	Hexacosane	366	C26H54	000630-01-3	80
4	Z-2-Tridecen-1-ol	198	C13H26O	1000130-75-8	74
5	Tetracosane	338	C24H50	000646-31-1	64

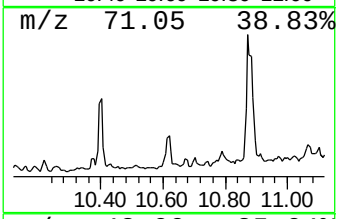


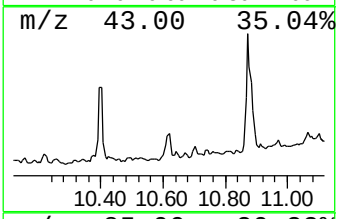


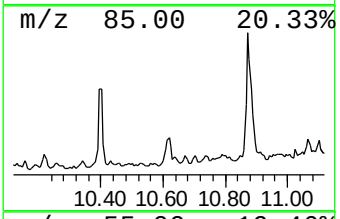


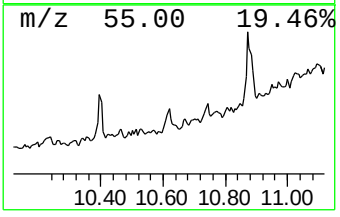












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

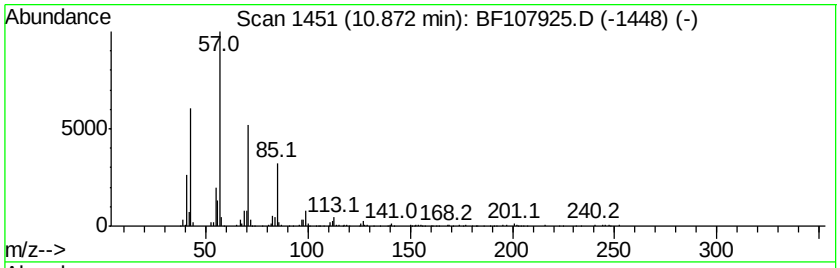
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

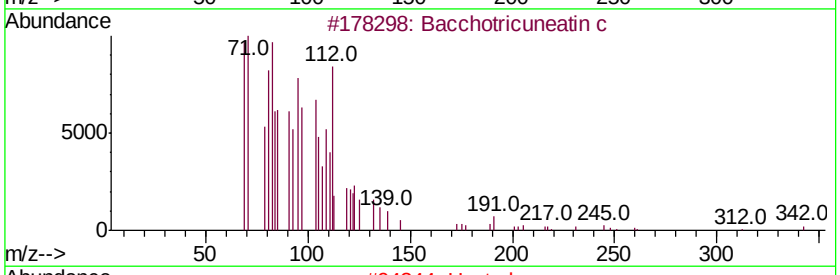
****

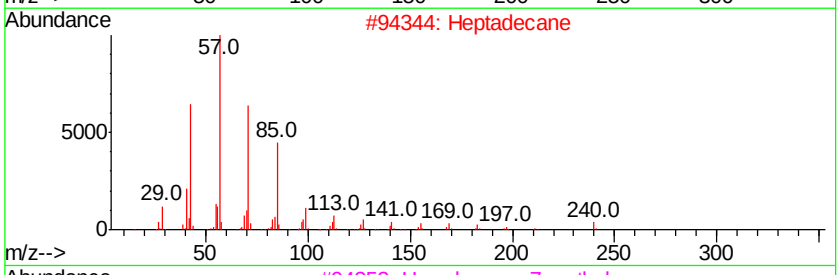
Peak Number 9 Bacchotricuneatin c Concentration Rank 3

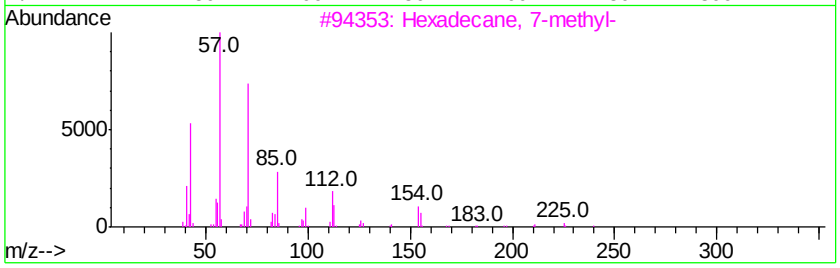
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.87	12.71 ng	373445	Phenanthrene-d10	11.49

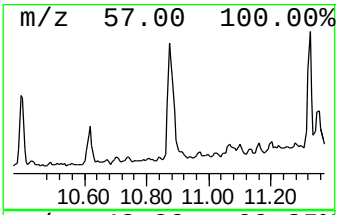
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bacchotricuneatin c	342	C20H22O5	066563-30-2	99
2	Heptadecane	240	C17H36	000629-78-7	94
3	Hexadecane, 7-methyl-	240	C17H36	026730-20-1	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	87

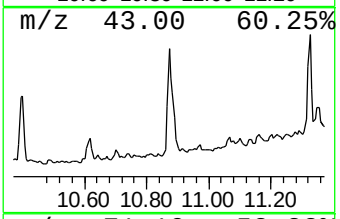


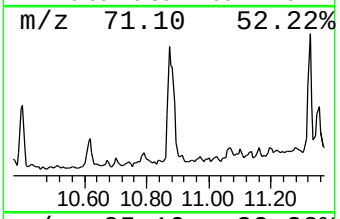


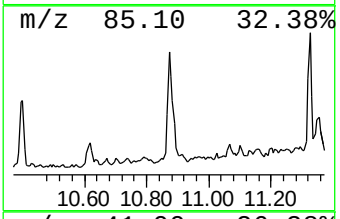


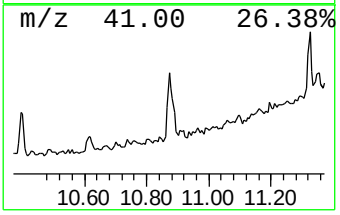












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080218\
Data File : BF107925.D
Acq On : 2 Aug 2018 22:28
Operator : JU/SJ
Sample : J4285-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KG-PIT-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

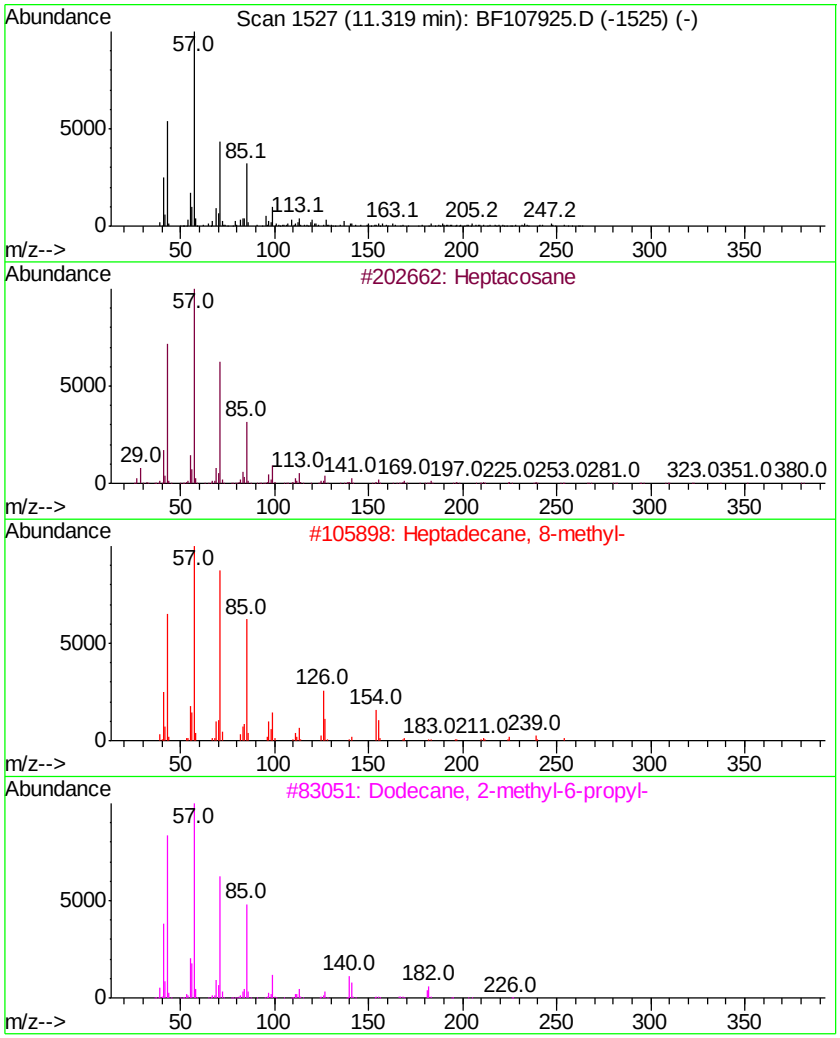
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

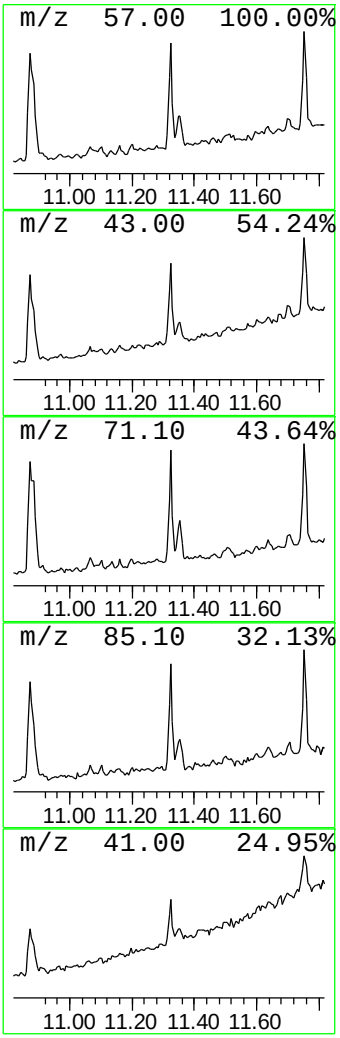
****

Peak Number 10 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.32	9.01 ng	264737	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	90
3	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	90
4	Heptadecane	240	C17H36	000629-78-7	86
5	Pentadecane	212	C15H32	000629-62-9	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF080218\
Data File : BF107925.D
Acq On : 2 Aug 2018 22:28
Operator : JU/SJ
Sample : J4285-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KG-PIT-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.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
2-Pentanone, 4-hy...	5.18	9.6	ng	334125	1	6.95	692969	20.0
unknown6.73	6.73	68.5	ng	2373410	1	6.95	692969	20.0
Naphthalene, 1-me...	9.05	3.3	ng	164765	2	8.24	1001620	20.0
Undecane	9.37	2.6	ng	96198	3	9.99	747445	20.0
Hexadecane	9.90	2.9	ng	108411	3	9.99	747445	20.0
Pentadecane	10.40	5.5	ng	206903	3	9.99	747445	20.0
Pentadecane, 2,6,...	10.62	2.4	ng	87650	3	9.99	747445	20.0
Bacchotricuneatin c	10.87	12.7	ng	373445	4	11.49	587719	20.0
Heptacosane	11.32	9.0	ng	264737	4	11.49	587719	20.0