LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080118\
Data File : BF107895.D
Acq On : 1 Aug 2018 18:01
Operator : JU/SJ
Sample : J4256-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-25

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	481	484	497	rBV	211469	268475	7.18%	0.953%
2	5.596	551	554	573	rBV	690941	1322823	35.36%	4.697%
3	6.601	722	725	744	rBV	345066	947435	25.33%	3.364%
4	6.737	744	748	769	rVV	2206286	2864590	76.58%	10.172%
5	6.966	783	787	806	rVB	373006	704961	18.85%	2.503%
6	7.113	809	812	829	rBV	2225146	2741105	73.28%	9.734%
7	7.531	879	883	900	rBV	1211874	2091479	55.91%	7.427%
8	7.748	916	920	929	rVB	87355	117881	3.15%	0.419%
9	8.242	1001	1004	1009	rBV	591546	675579	18.06%	2.399%
10	9.313	1182	1186	1197	rBV	3162501	3709081	99.16%	13.171%
11	9.419	1201	1204	1209	rVB	105889	127646	3.41%	0.453%
12	9.707	1249	1253	1267	rBV	619377	664140	17.76%	2.358%
13	10.001	1299	1303	1314	rBV	863635	904208	24.17%	3.211%
14	10.372	1364	1366	1369	rBV2	35605	37982	1.02%	0.135%
15	10.407	1369	1372	1375	rVB2	45603	41762	1.12%	0.148%
16	10.795	1434	1438	1450	rBV	1709828	2338987	62.53%	8.306%
17	10.878	1450	1452	1456	rVB2	33596	51998	1.39%	0.185%
18	10.960	1463	1466	1469	rBV	60584	58250	1.56%	0.207%
19	10.989	1469	1471	1475	rVB2	57840	70350	1.88%	0.250%
20	11.030	1475	1478	1480	rBV2	55509	49526	1.32%	0.176%
21	11.142	1493	1497	1500	rVV3	75164	73973	1.98%	0.263%
22	11.178	1500	1503	1505	rVV	60933	51759	1.38%	0.184%
23	11.330	1526	1529	1532	rBV2	52118	52536	1.40%	0.187%
24	11.383	1536	1538	1548	rVB	42788	66224	1.77%	0.235%
25	11.495	1554	1557	1569	rBV	660281	916368	24.50%	3.254%
26	11.701	1590	1592	1596	rVV3	43012	45427	1.21%	0.161%
27	11.760	1599	1602	1607	rVB	35967	40566	1.08%	0.144%
28	11.866	1617	1620	1625	rBV2	75914	79074	2.11%	0.281%
29	12.001	1640	1643	1653	rBV2	221812	301320	8.06%	1.070%
30	12.525	1728	1732	1736	rBV	228025	273246	7.31%	0.970%
31	12.789	1775	1777	1782	rBV5	39054	49098	1.31%	0.174%
32	13.083	1822	1827	1851	rBV	3036131	3740504	100.00%	13.283%
33	13.272	1857	1859	1864	rBV2	51326	69590	1.86%	0.247%
34	13.513	1897	1900	1903	rBV	100864	96351	2.58%	0.342%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080118\
Data File : BF107895.D
Acq On : 1 Aug 2018 18:01
Operator : JU/SJ
Sample : J4256-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-25

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

35	13.566	1907	1909	1916	rVB6	67009	96548	2.58%	0.343%
36	13.624	1917	1919	1923	rBV3	42618	44980	1.20%	0.160%
37	13.960	1973	1976	1985	rBV	333311	383510	10.25%	1.362%
38	14.095	1997	1999	2003	rBV	65328	58441	1.56%	0.208%
39	14.154	2005	2009	2019	rBV	677388	972271	25.99%	3.453%
40	14.977	2147	2149	2154	rVB	62730	60485	1.62%	0.215%
41	15.689	2266	2270	2282	rVB	515323	899787	24.06%	3.195%

Sum of corrected areas: 28160316

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080118\
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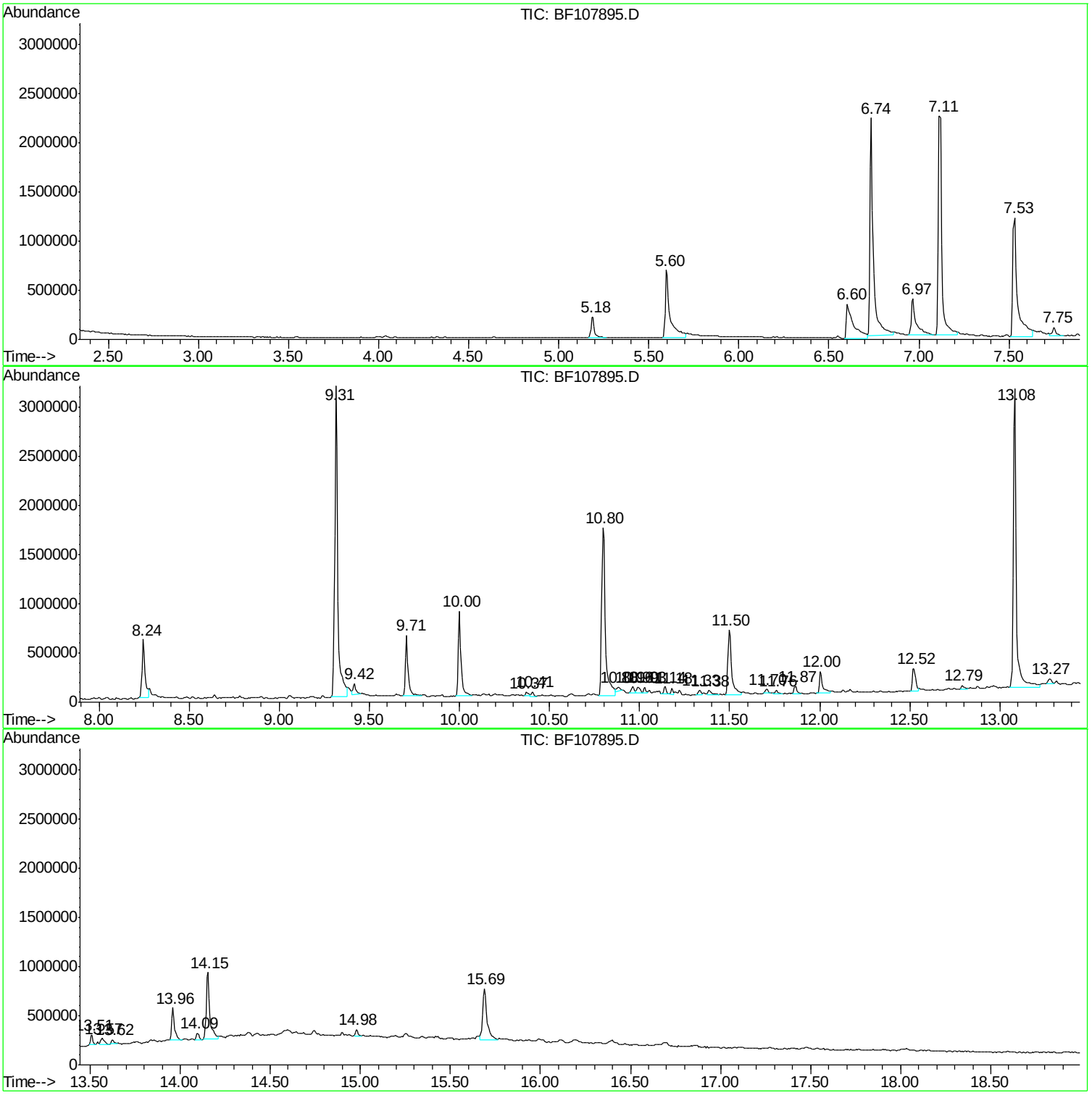
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-25

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

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080118\
Data File : BF107895.D
Acq On : 1 Aug 2018 18:01
Operator : JU/SJ
Sample : J4256-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-25

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

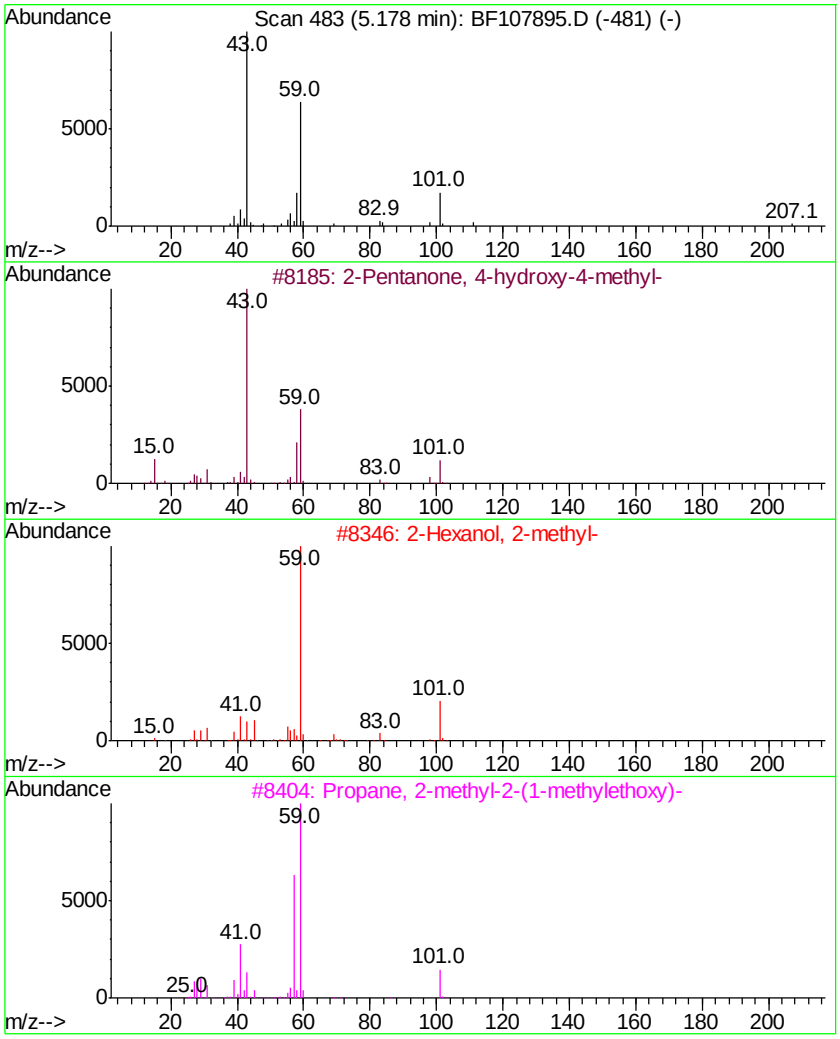
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

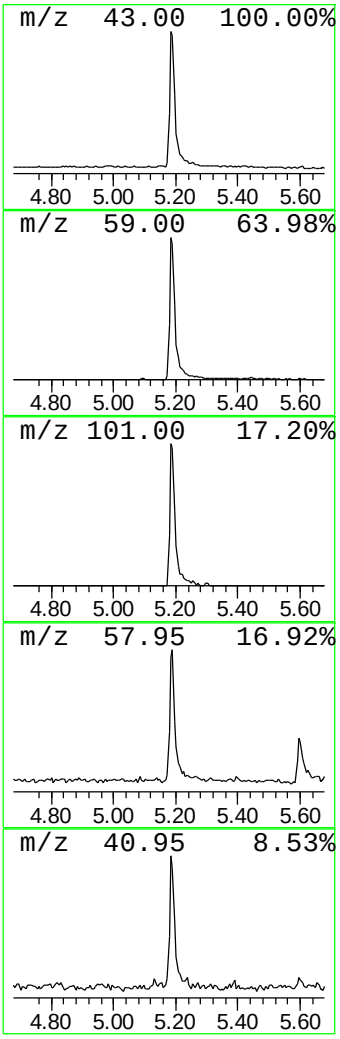
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	7.62 ng	268475	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080118\
Data File : BF107895.D
Acq On : 1 Aug 2018 18:01
Operator : JU/SJ
Sample : J4256-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-25

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

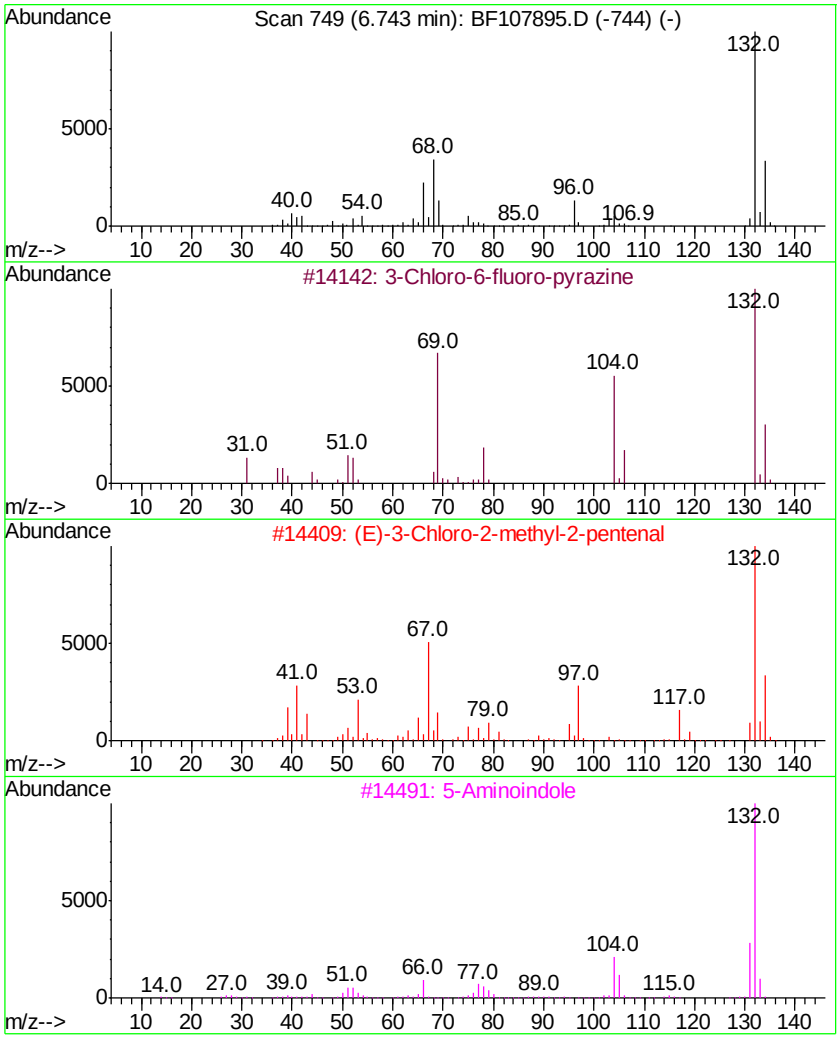
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

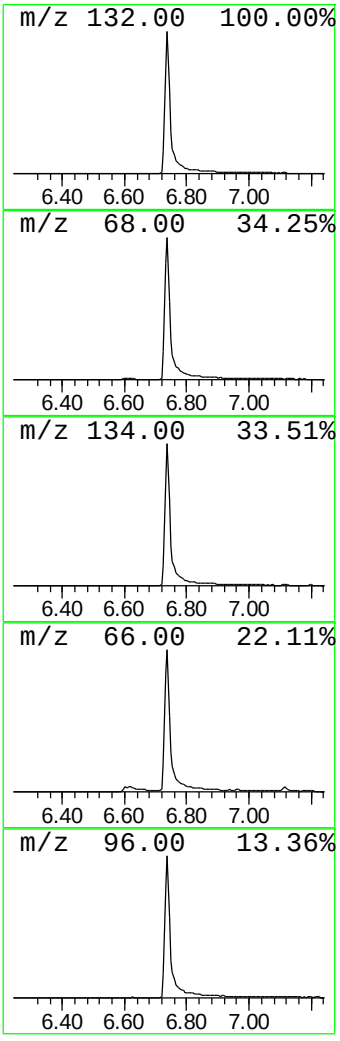
****

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	81.27 ng	2864590	1,4-Dichlorobenzene-d4	6.97

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	35
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080118\
Data File : BF107895.D
Acq On : 1 Aug 2018 18:01
Operator : JU/SJ
Sample : J4256-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-25

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

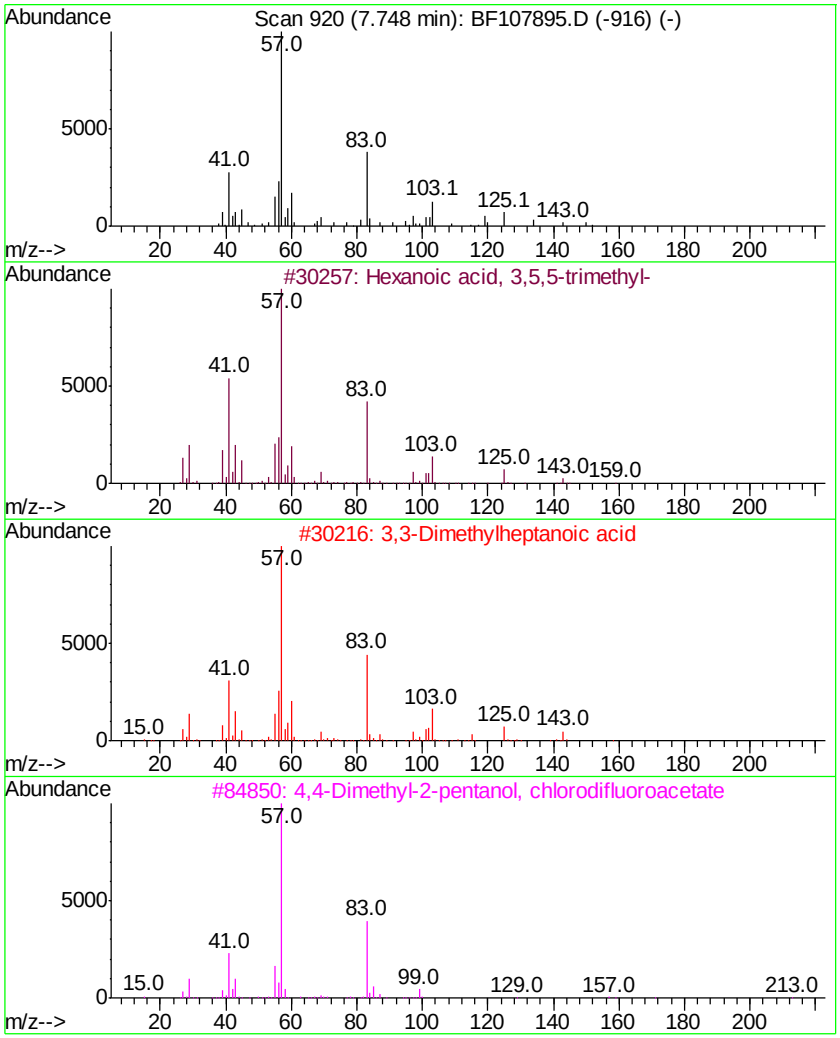
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

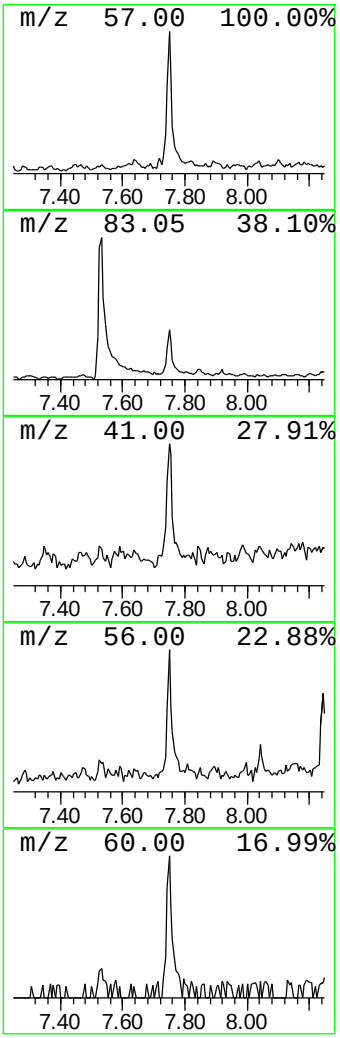
****

Peak Number 4 Hexanoic acid, 3,5,5-trimet... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.75	3.49 ng	117881	Naphthalene-d8	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	86
2	3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	50
3	4,4-Dimethyl-2-pentanol, chlorod...	228	C9H15ClF2O2	1000376-27-0	38
4	Formic acid, 4,4-dimethylpent-2-...	144	C8H16O2	1000368-69-9	37
5	Hexanoyl chloride, 3,5,5-trimethyl-	176	C9H17ClO	036727-29-4	28





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080118\
Data File : BF107895.D
Acq On : 1 Aug 2018 18:01
Operator : JU/SJ
Sample : J4256-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-25

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

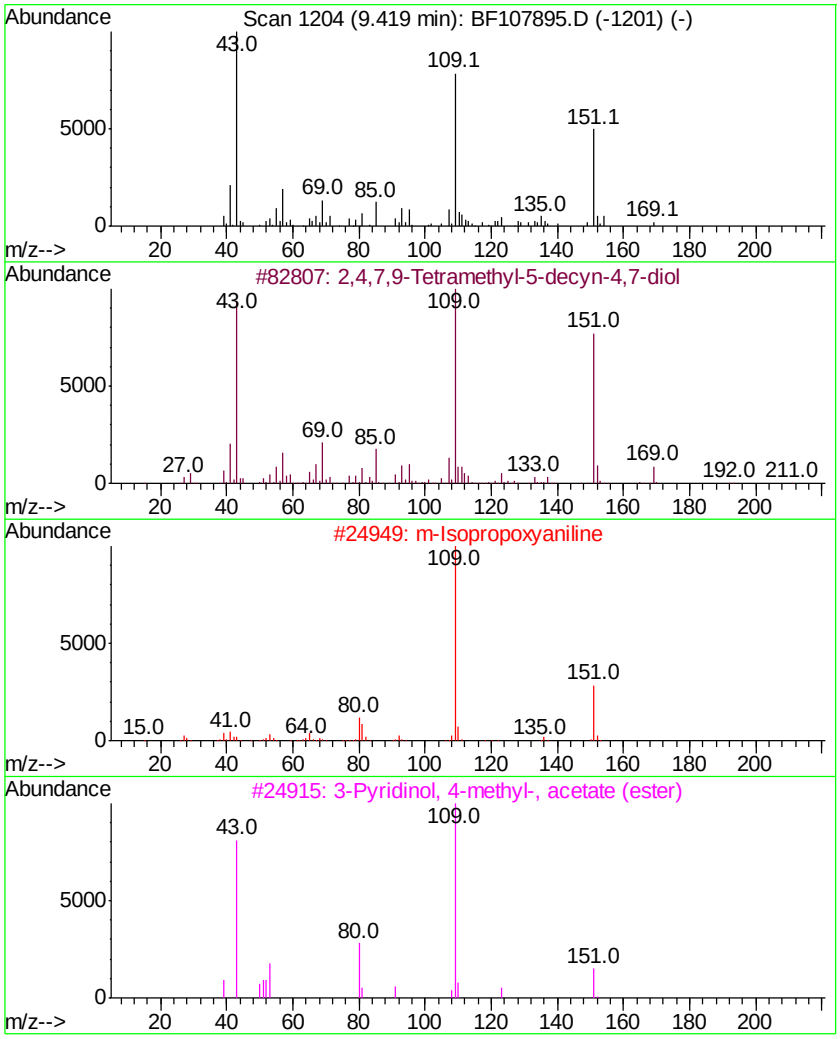
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

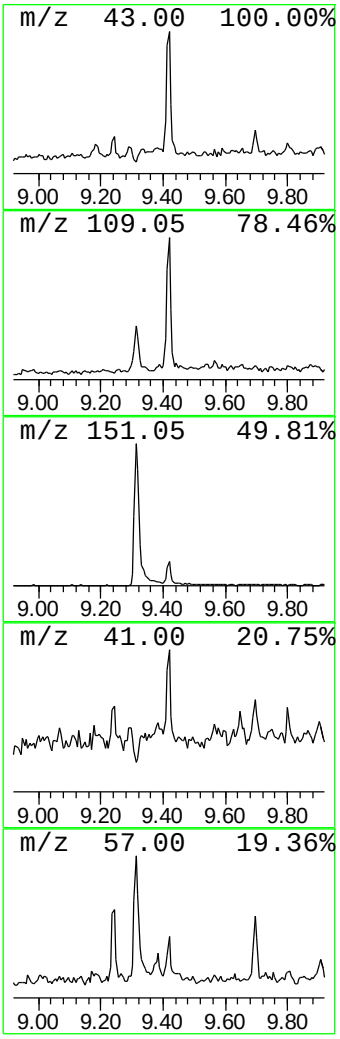
****

Peak Number 5 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.42	2.82 ng	127646	Acenaphthene-d10	10.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87
2	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	64
3	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	64
4	Metacetamol	151	C8H9NO2	000621-42-1	64
5	Pyridine, 3-butyl-, 1-oxide	151	C9H13NO	031396-33-5	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080118\
Data File : BF107895.D
Acq On : 1 Aug 2018 18:01
Operator : JU/SJ
Sample : J4256-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-25

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

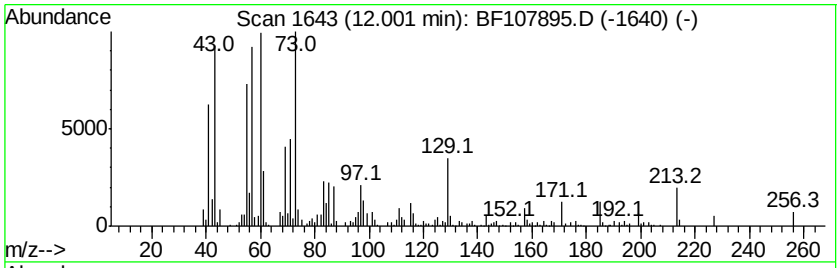
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

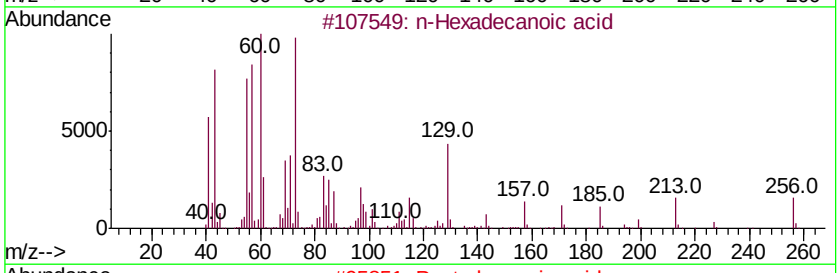
****

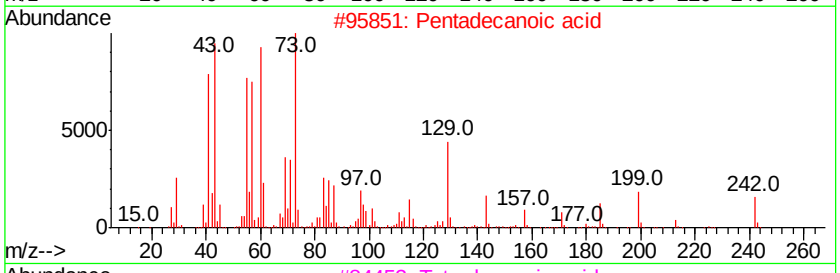
Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

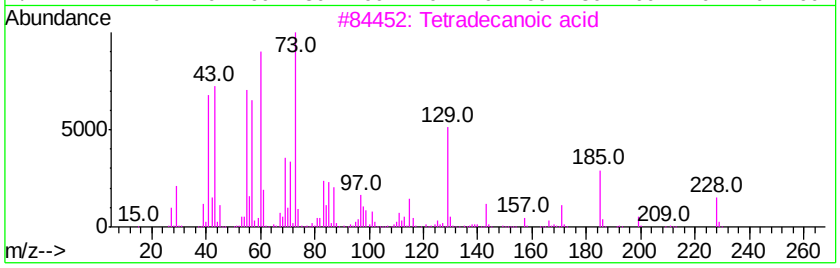
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	6.58 ng	301320	Phenanthrene-d10	11.50

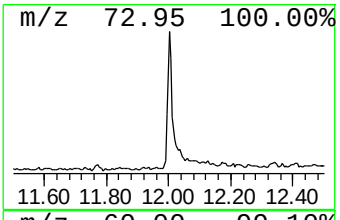
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64

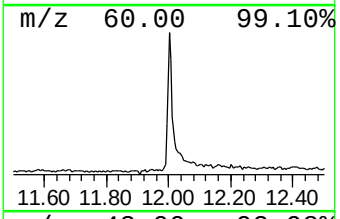


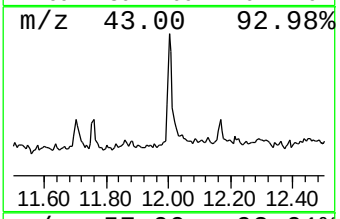


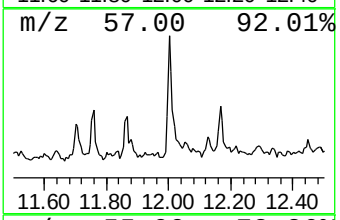


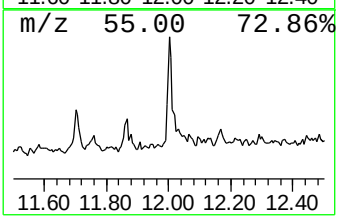












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080118\
Data File : BF107895.D
Acq On : 1 Aug 2018 18:01
Operator : JU/SJ
Sample : J4256-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-25

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

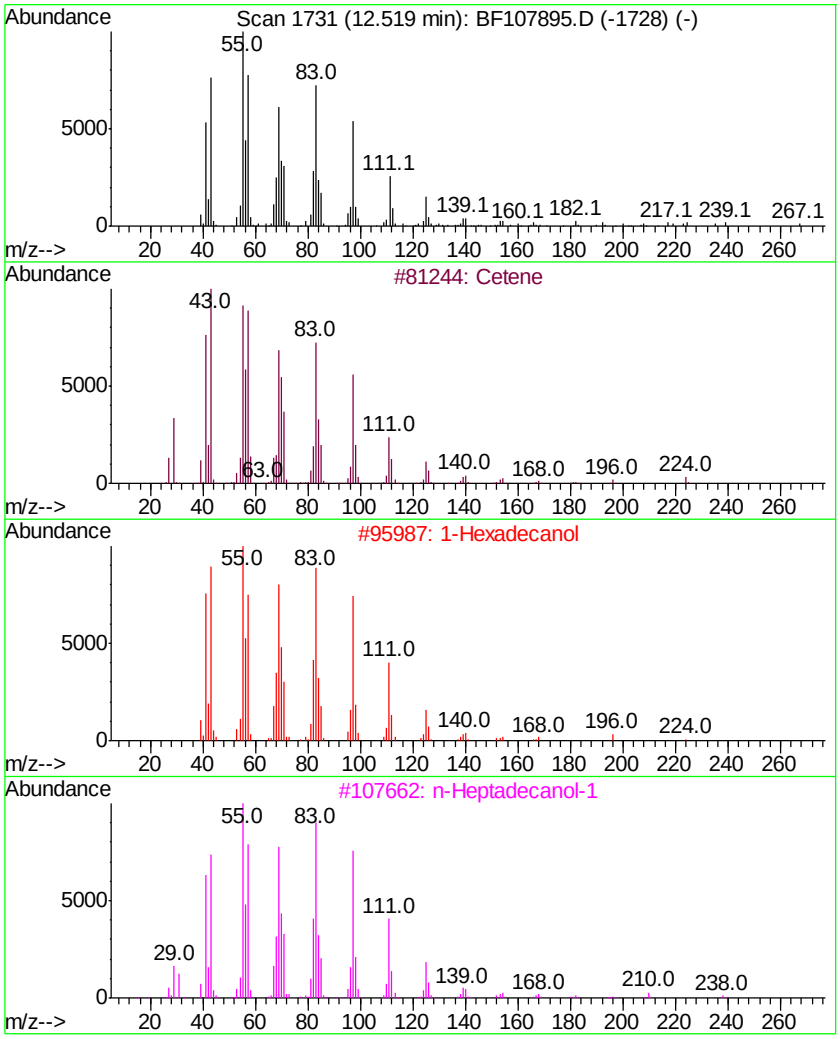
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

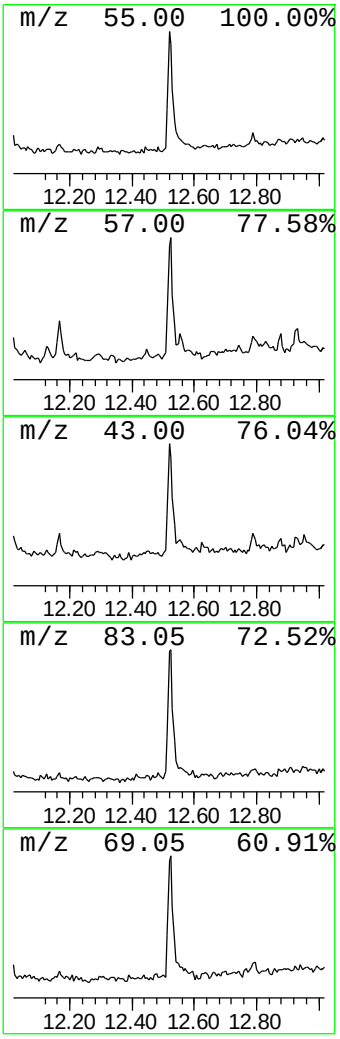
****

Peak Number 7 Cetene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.52	5.96 ng	273246	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cetene	224	C16H32	000629-73-2	96
2	1-Hexadecanol	242	C16H34O	036653-82-4	91
3	n-Heptadecanol-1	256	C17H36O	001454-85-9	91
4	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
5	E-14-Hexadecenal	238	C16H30O	330207-53-9	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080118\
Data File : BF107895.D
Acq On : 1 Aug 2018 18:01
Operator : JU/SJ
Sample : J4256-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-25

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

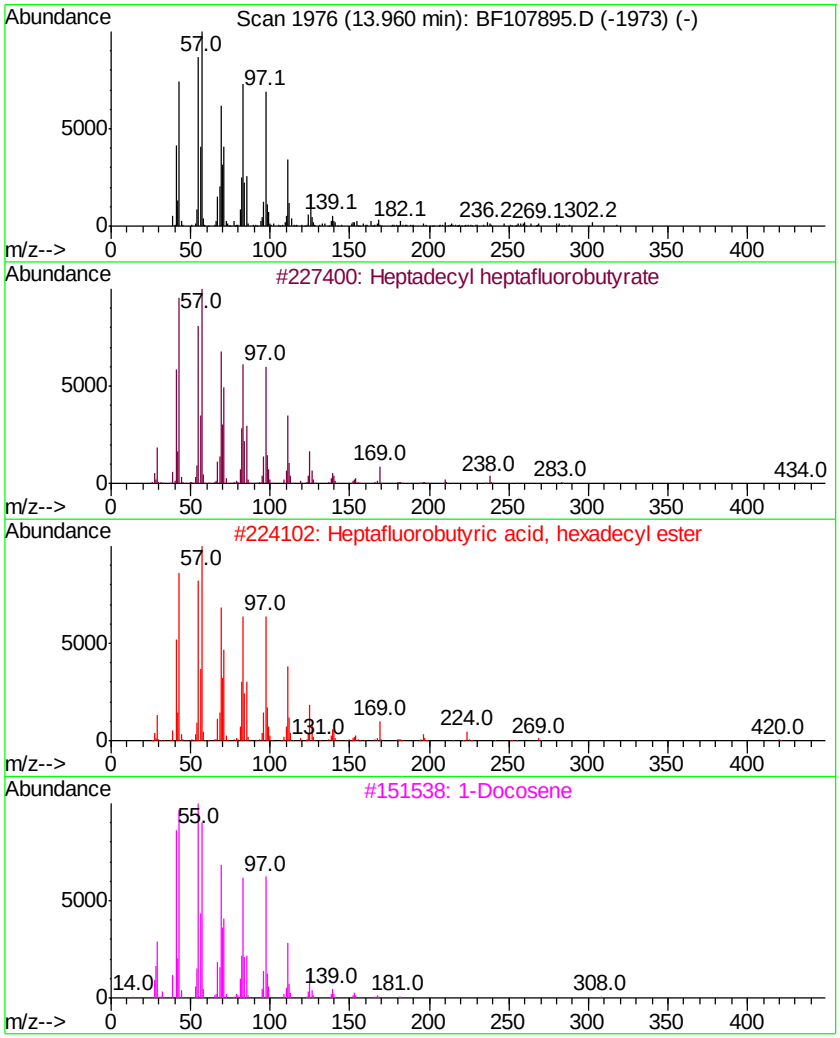
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

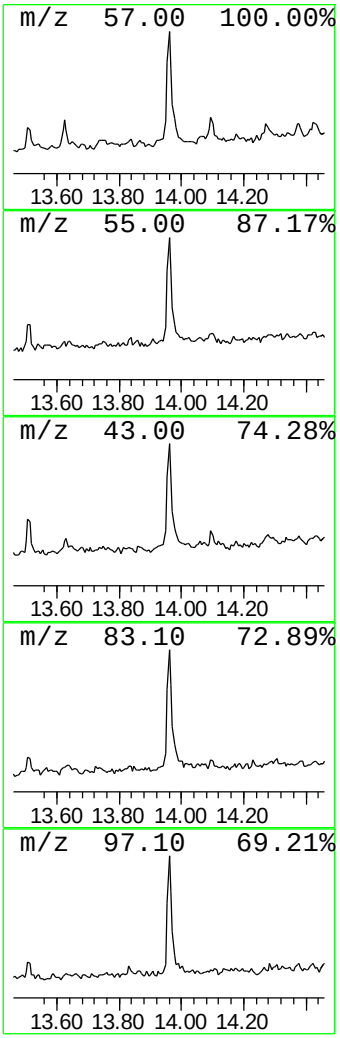
****

Peak Number 8 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	7.89 ng	383510	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
3	1-Docosene	308	C22H44	001599-67-3	91
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
5	11-Tricosene	322	C23H46	052078-56-5	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF080118\
Data File : BF107895.D
Acq On : 1 Aug 2018 18:01
Operator : JU/SJ
Sample : J4256-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-25

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	7.6	ng	268475	1	6.97	704961	20.0
unknown6.74	6.74	81.3	ng	2864590	1	6.97	704961	20.0
Hexanoic acid, 3,...	7.75	3.5	ng	117881	2	8.24	675579	20.0
2,4,7,9-Tetrameth...	9.42	2.8	ng	127646	3	10.00	904208	20.0
n-Hexadecanoic acid	12.00	6.6	ng	301320	4	11.50	916368	20.0
Cetene	12.52	6.0	ng	273246	4	11.50	916368	20.0
Heptadecyl heptaf...	13.96	7.9	ng	383510	5	14.15	972271	20.0