LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081418\
Data File : BF108155.D
Acq On : 14 Aug 2018 19:56
Operator : JU/SJ
Sample : J4458-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-94

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-BF080818.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	2.372	3	6	15	rVB	1720485	2175716	60.14%	7.536%
2	2.501	25	28	35	rVB2	30471	40951	1.13%	0.142%
3	3.660	222	225	233	rBV	19910	40497	1.12%	0.140%
4	4.907	433	437	441	rVB	35524	39614	1.10%	0.137%
5	5.254	492	496	502	rVB	116307	117773	3.26%	0.408%
6	5.642	558	562	566	rBV	1066205	907043	25.07%	3.142%
7	6.589	718	723	726	rBV	29308	39217	1.08%	0.136%
8	6.631	726	730	742	rVB	665646	604008	16.70%	2.092%
9	6.783	752	756	760	rBV	1999192	1661208	45.92%	5.754%
10	6.831	761	764	770	rVB	43401	40948	1.13%	0.142%
11	7.019	792	796	799	rBV	1357105	1115882	30.85%	3.865%
12	7.178	818	823	826	rVB	2979869	2833429	78.33%	9.814%
13	7.578	886	891	894	rBV	2372569	2234578	61.77%	7.740%
14	7.642	897	902	906	rVB	42317	46833	1.29%	0.162%
15	8.301	1010	1014	1017	rBV	1511064	1253995	34.66%	4.343%
16	8.842	1102	1106	1110	rBV2	46304	46376	1.28%	0.161%
17	9.372	1189	1196	1200	rBV	3851003	3617469	100.00%	12.530%
18	9.472	1210	1213	1216	rVB2	40863	42385	1.17%	0.147%
19	9.766	1258	1263	1266	rBV	632958	519888	14.37%	1.801%
20	9.848	1274	1277	1284	rVB5	29207	41280	1.14%	0.143%
21	9.972	1293	1298	1304	rBV5	25499	41999	1.16%	0.145%
22	10.066	1309	1314	1320	rVB	1323199	1220567	33.74%	4.228%
23	10.242	1339	1344	1346	rBV4	39146	46565	1.29%	0.161%
24	10.471	1381	1383	1386	rVB2	88169	67812	1.87%	0.235%
25	10.695	1417	1421	1423	rBV	34776	39374	1.09%	0.136%
26	10.854	1444	1448	1452	rBV	1302235	1122677	31.03%	3.889%
27	10.948	1461	1464	1471	rVB3	111219	145120	4.01%	0.503%
28	11.024	1474	1477	1479	rBV	58375	48689	1.35%	0.169%
29	11.054	1479	1482	1486	rBV2	64204	63229	1.75%	0.219%
30	11.089	1486	1488	1491	rBV2	54160	53218	1.47%	0.184%
31	11.201	1504	1507	1511	rVB3	55841	78742	2.18%	0.273%
32	11.242	1511	1514	1515	rBV2	64929	60640	1.68%	0.210%
33	11.395	1538	1540	1543	rBV	73570	72647	2.01%	0.252%
34	11.560	1564	1568	1571	rBV	1420500	1187913	32.84%	4.115%

LSC Area Percent Report

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Sample : J4458-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-94

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-BF080818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.930	1629	1631	1634	rVB3	52714	39559	1.09%	0.137%
36	12.071	1651	1655	1663	rBV2	422820	505733	13.98%	1.752%
37	12.577	1739	1741	1745	rVB	117691	105231	2.91%	0.364%
38	12.860	1786	1789	1794	rBV3	103760	146088	4.04%	0.506%
39	13.148	1834	1838	1841	rBV	3609318	3070288	84.87%	10.634%
40	14.030	1985	1988	1994	rBV	682679	666018	18.41%	2.307%
41	14.218	2016	2020	2023	rVB	1274047	1127728	31.17%	3.906%
42	14.983	2148	2150	2154	rVB	173411	164225	4.54%	0.569%
43	15.354	2210	2213	2217	rVB	187067	214595	5.93%	0.743%
44	15.783	2280	2286	2291	rVB2	598025	966971	26.73%	3.349%
45	16.248	2362	2365	2371	rVB	131069	196459	5.43%	0.680%

Sum of corrected areas: 28871177

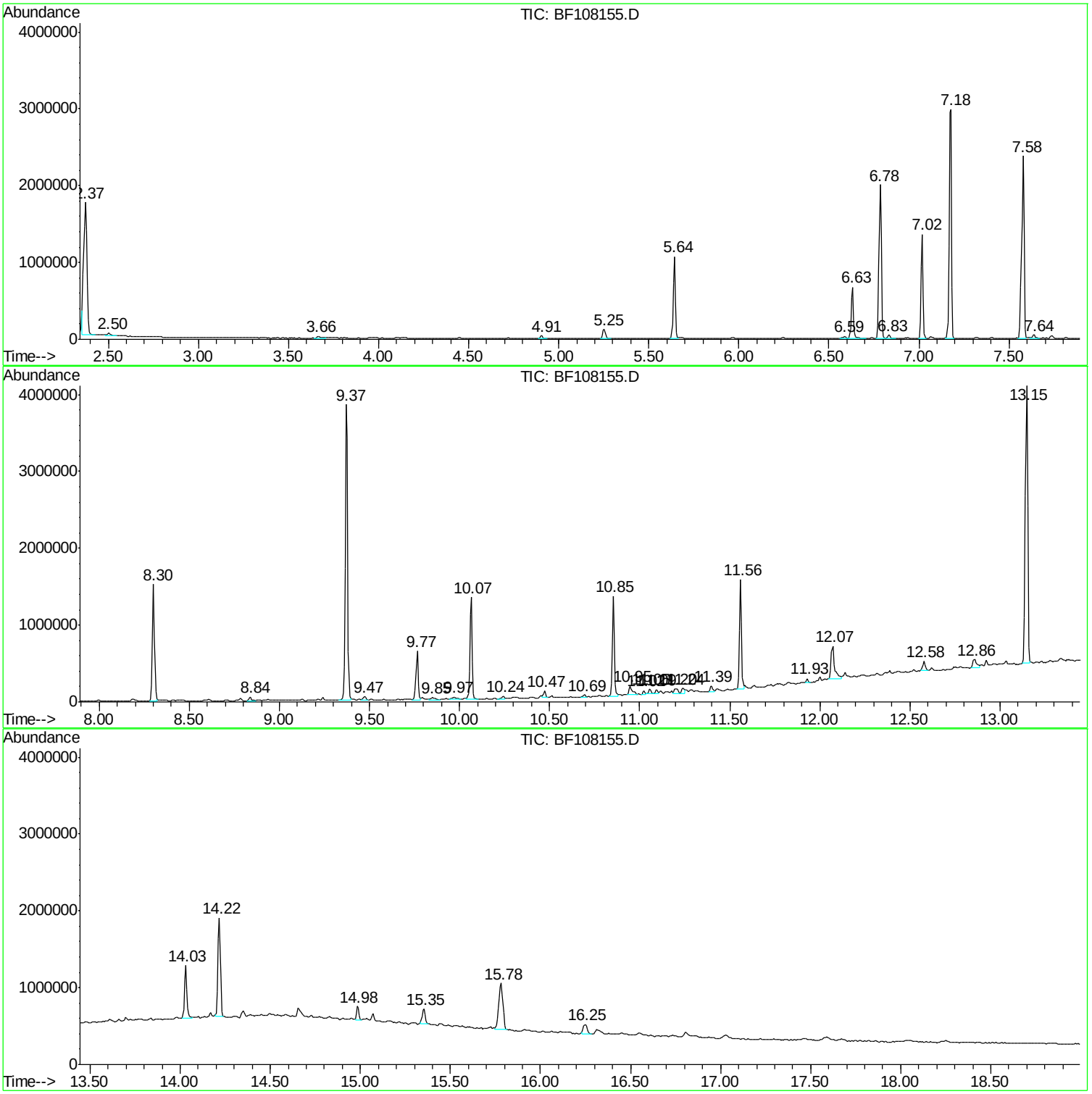
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081418\
Data File : BF108155.D
Acq On : 14 Aug 2018 19:56
Operator : JU/SJ
Sample : J4458-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-94

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081418\
Data File : BF108155.D
Acq On : 14 Aug 2018 19:56
Operator : JU/SJ
Sample : J4458-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-94

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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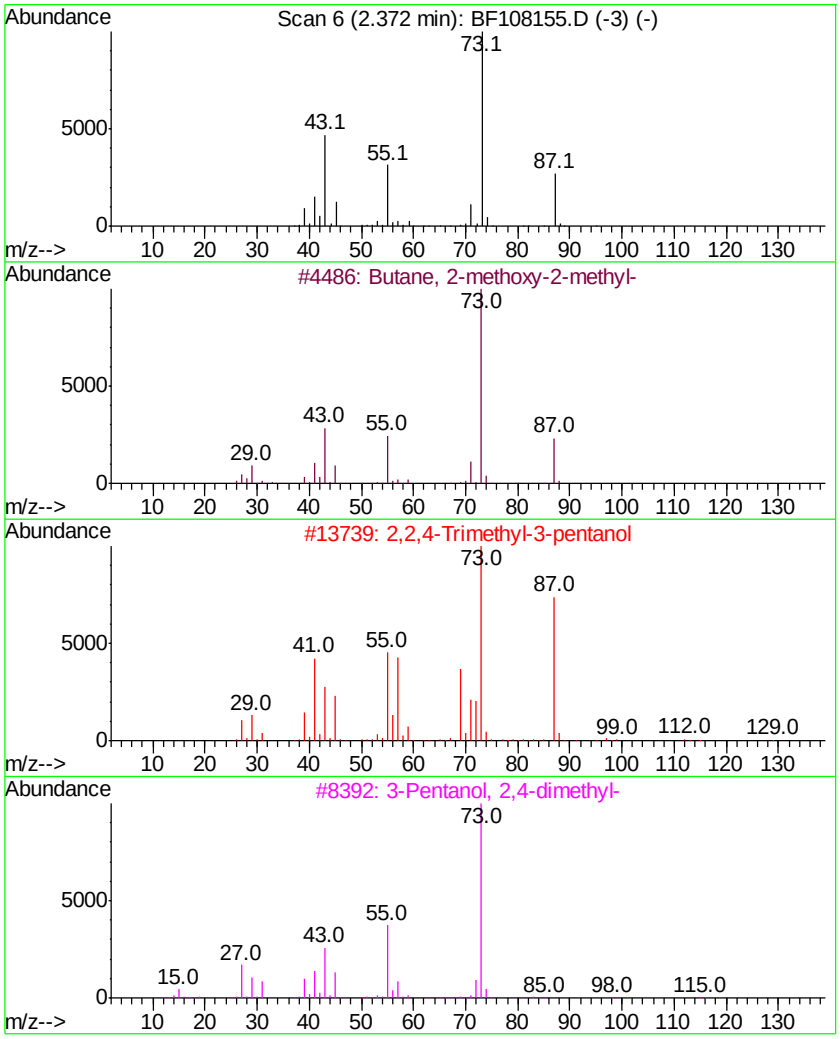
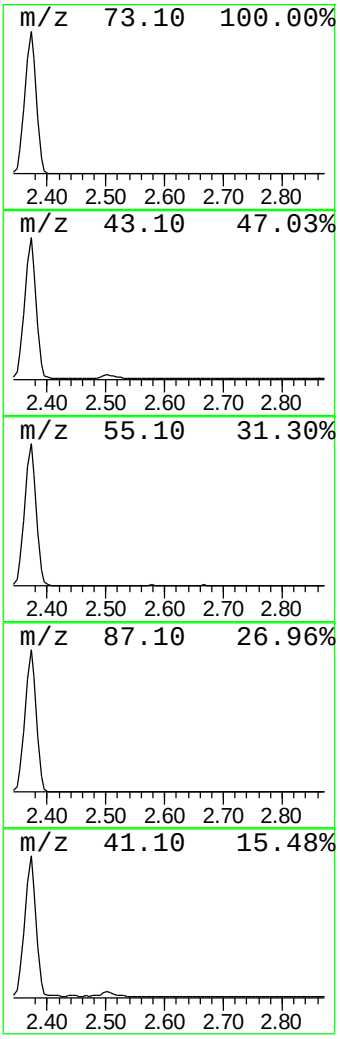
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.37	39.00 ng	2175720	1,4-Dichlorobenzene-d4	7.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081418\
Data File : BF108155.D
Acq On : 14 Aug 2018 19:56
Operator : JU/SJ
Sample : J4458-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-94

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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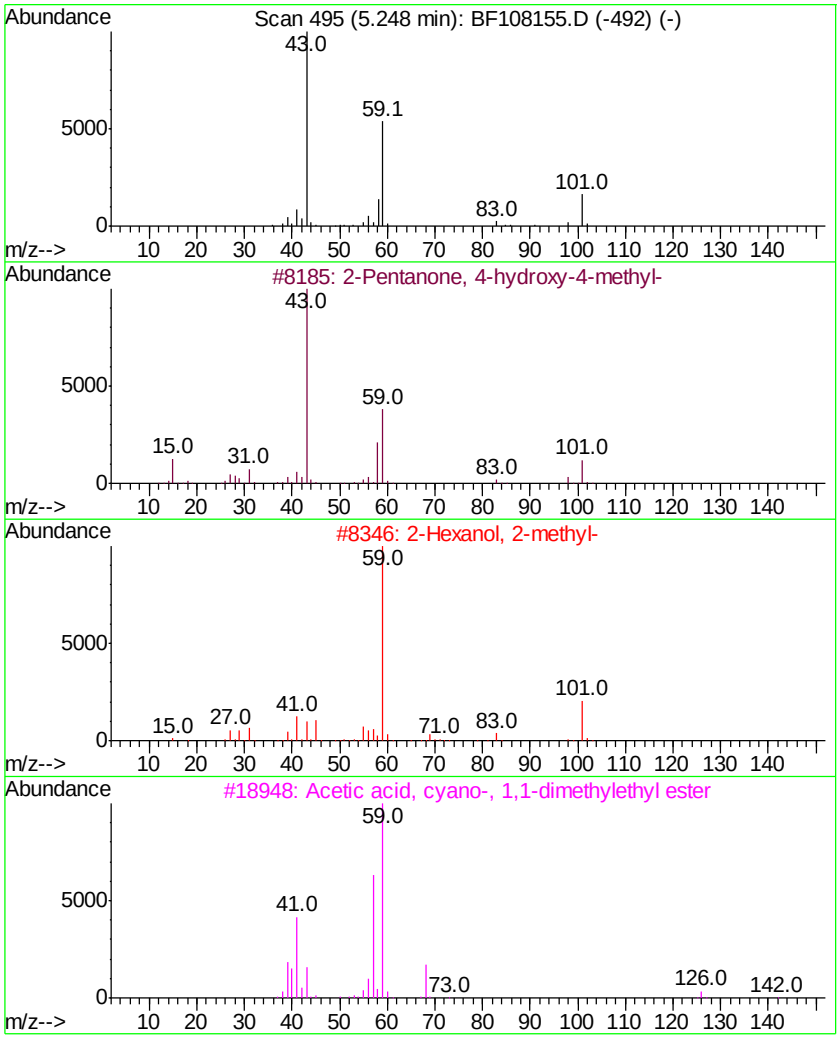
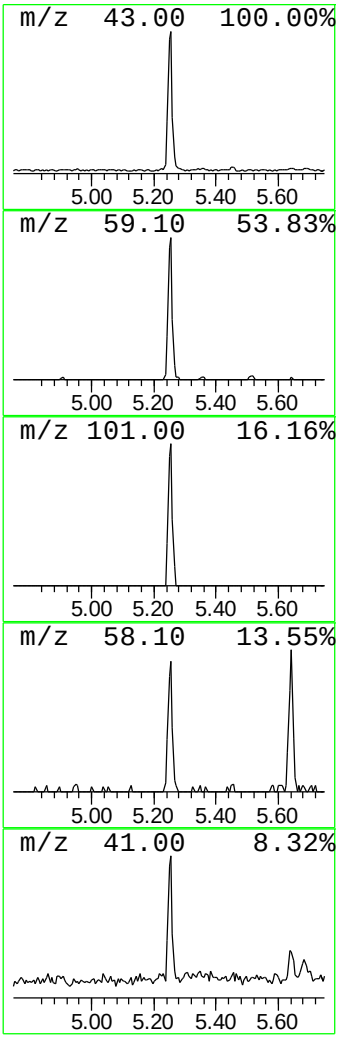
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.25	2.11 ng	117773	1,4-Dichlorobenzene-d4	7.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





Library Search Compound Report

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Data File : BF108155.D
Acq On : 14 Aug 2018 19:56
Operator : JU/SJ
Sample : J4458-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-94

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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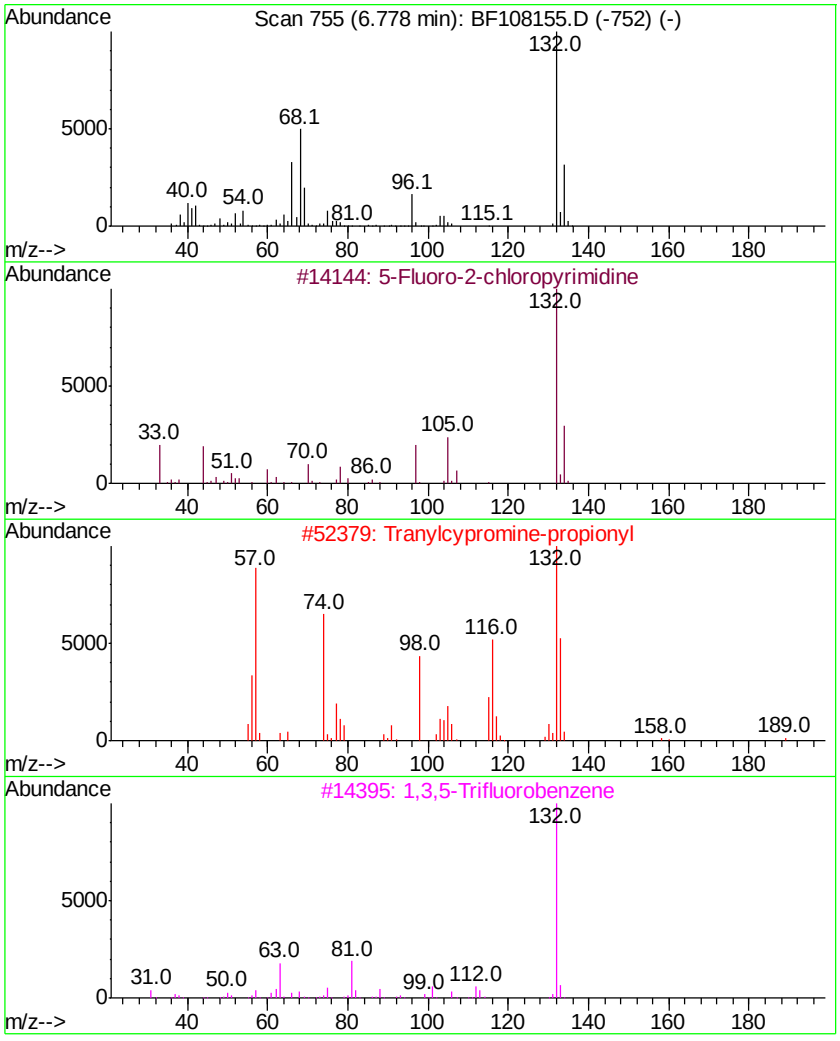
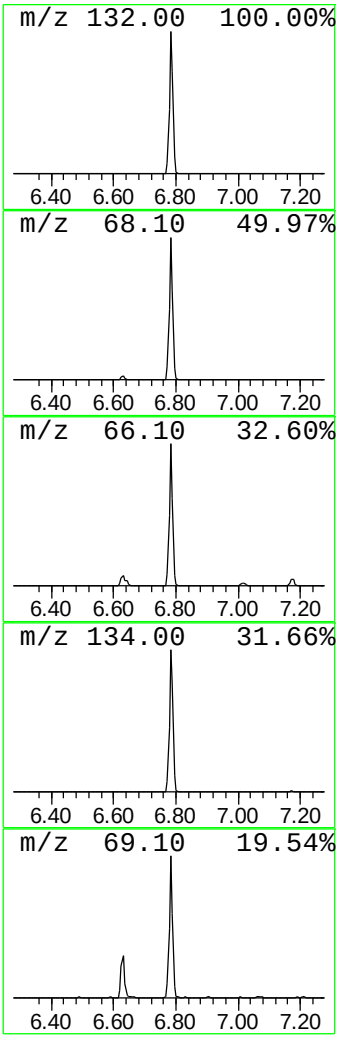
Peak Number 3 unknown6.78 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	29.77 ng	1661210	1,4-Dichlorobenzene-d4	7.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	1,2,3-Trifluorobenzene	132	C6H3F3	001489-53-8	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Data File : BF108155.D
Acq On : 14 Aug 2018 19:56
Operator : JU/SJ
Sample : J4458-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-94

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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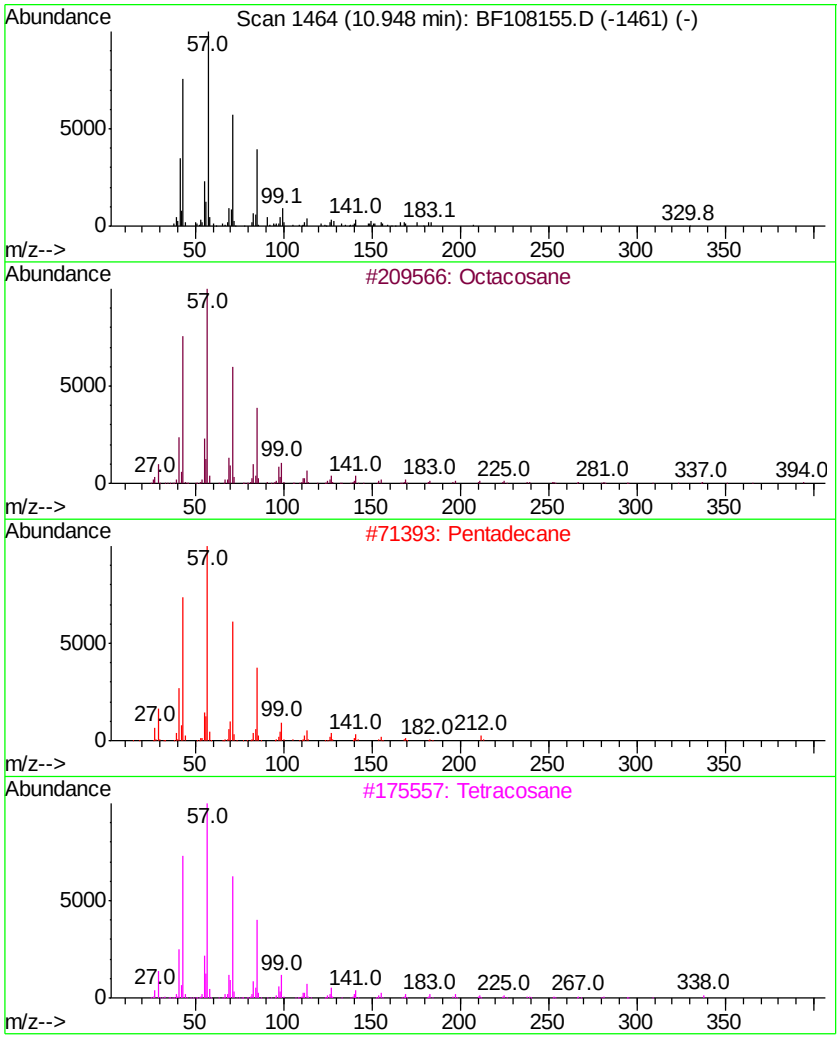
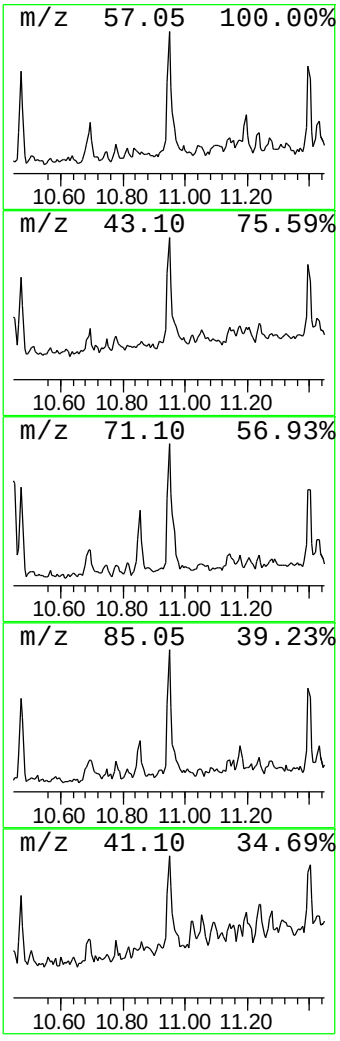
Peak Number 5 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.95	2.44 ng	145120	Phenanthrene-d10	11.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Pentadecane	212	C15H32	000629-62-9	83
3	Tetracosane	338	C24H50	000646-31-1	83
4	Tetradecane	198	C14H30	000629-59-4	80
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78





Library Search Compound Report

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Sample : J4458-03
Misc :
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Instrument : BNA_F
ClientSampleId : MH-94

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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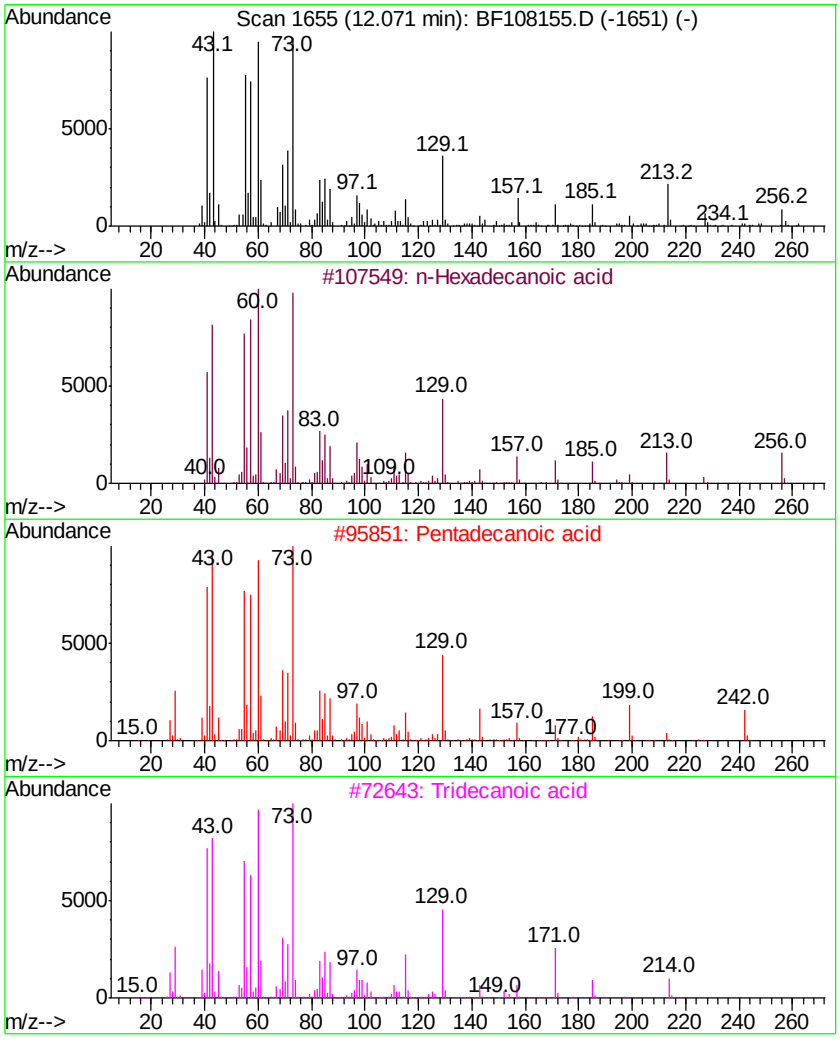
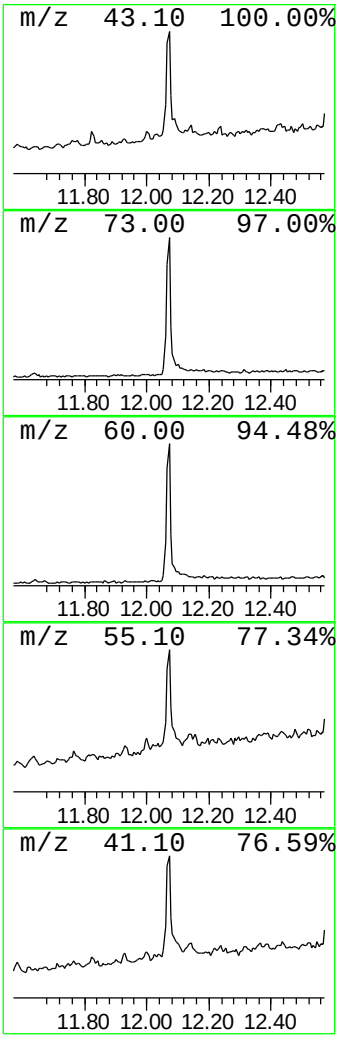
Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.07	8.51 ng	505733	Phenanthrene-d10	11.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	Undecanoic acid	186	C11H22O2	000112-37-8	74





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Instrument : BNA_F
ClientSampleId : MH-94

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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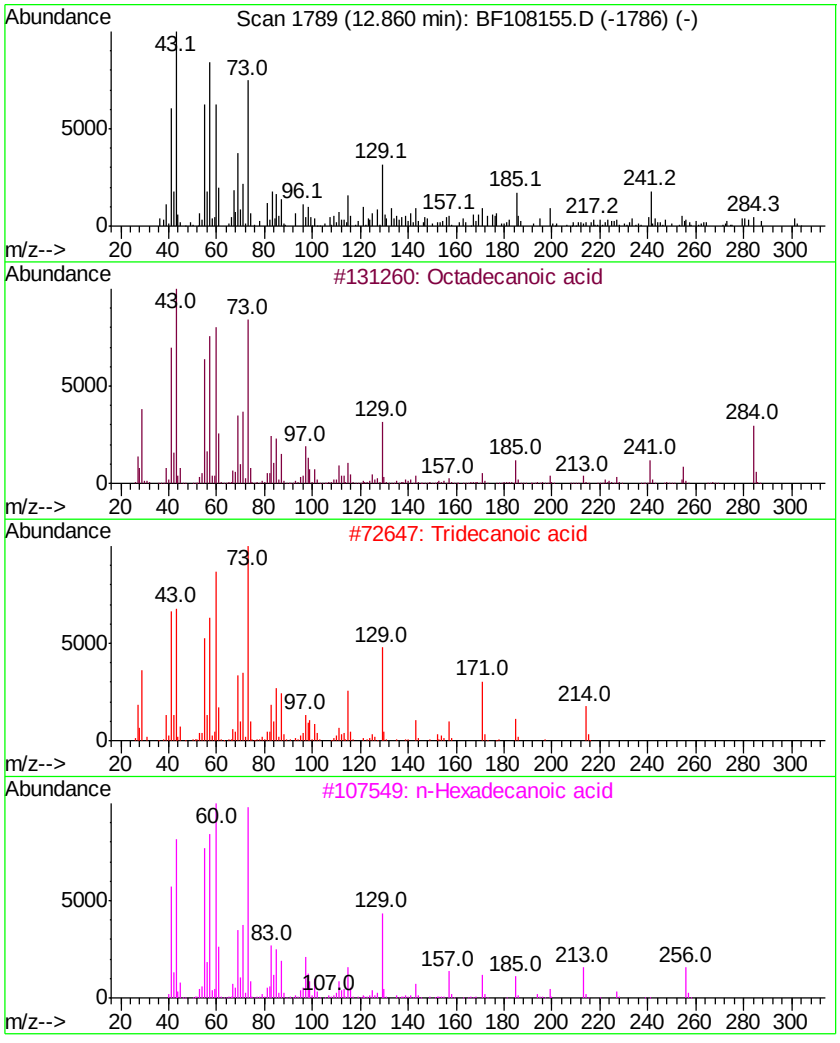
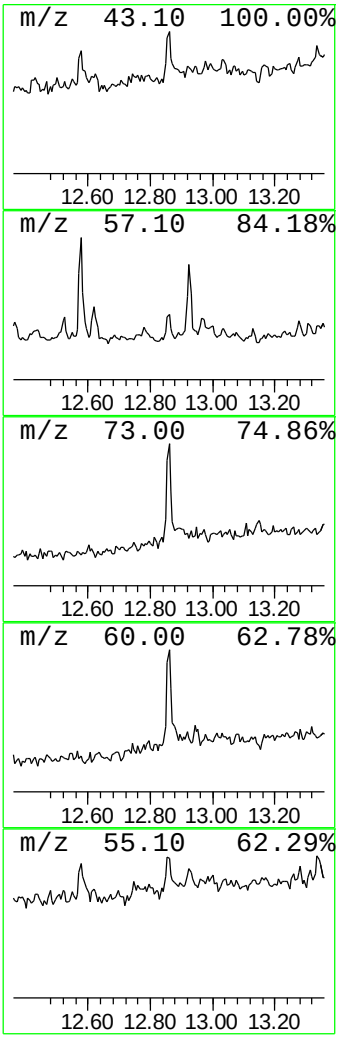
Peak Number 7 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.86	2.46 ng	146088	Phenanthrene-d10	11.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	72
2	Tridecanoic acid	214	C13H26O2	000638-53-9	64
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	59
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	52
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	52





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Misc :
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Instrument : BNA_F
ClientSampleId : MH-94

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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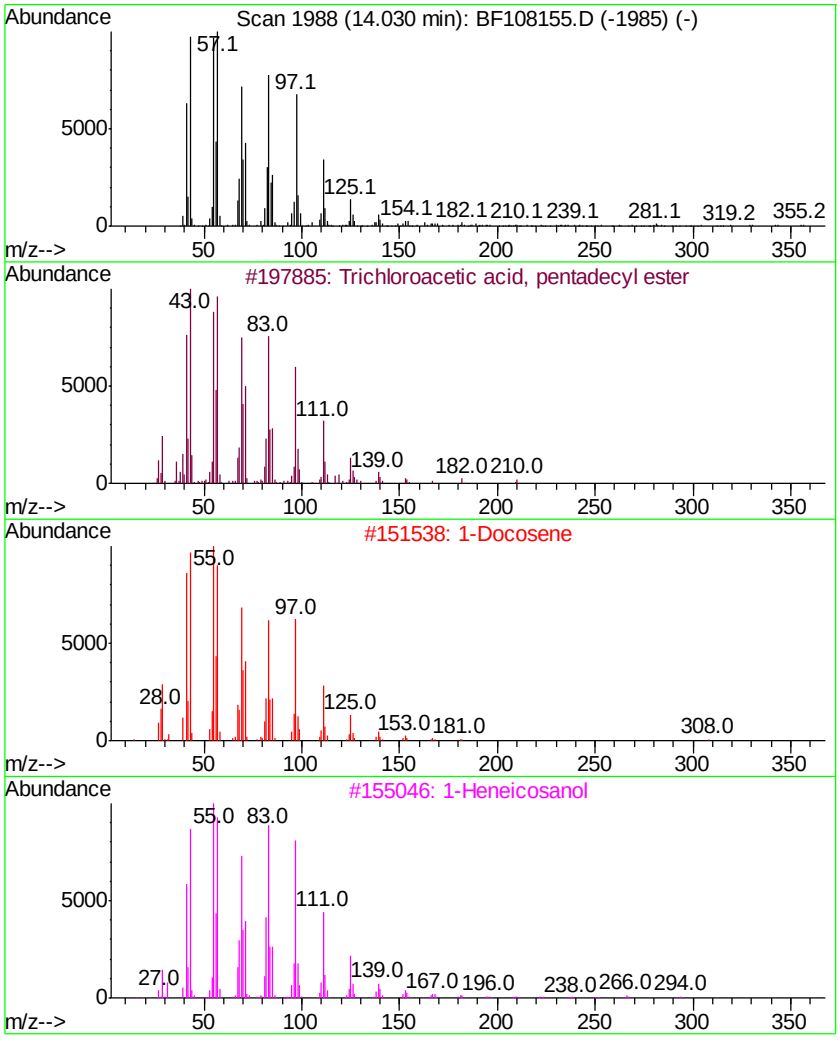
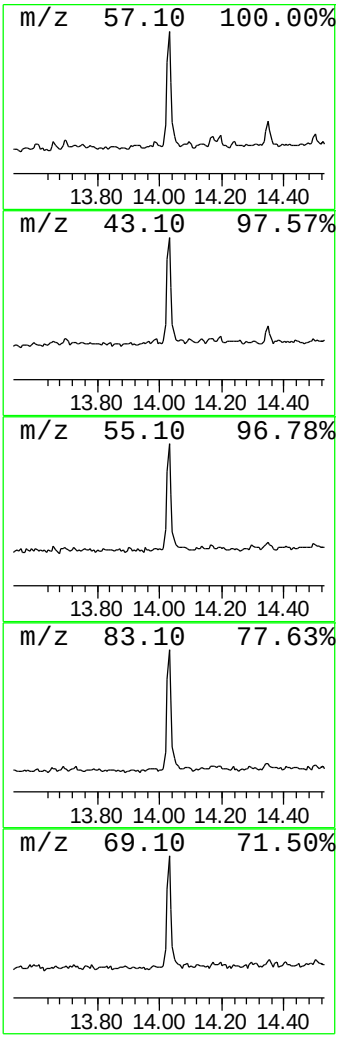
Peak Number 8 Trichloroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.03	11.81 ng	666018	Chrysene-d12	14.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
2	1-Docosene	308	C22H44	001599-67-3	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	94
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081418\
Data File : BF108155.D
Acq On : 14 Aug 2018 19:56
Operator : JU/SJ
Sample : J4458-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-94

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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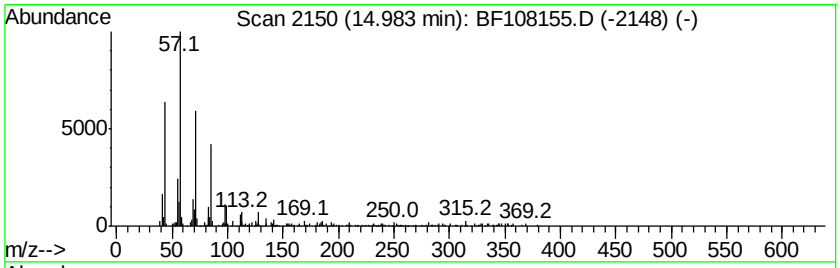
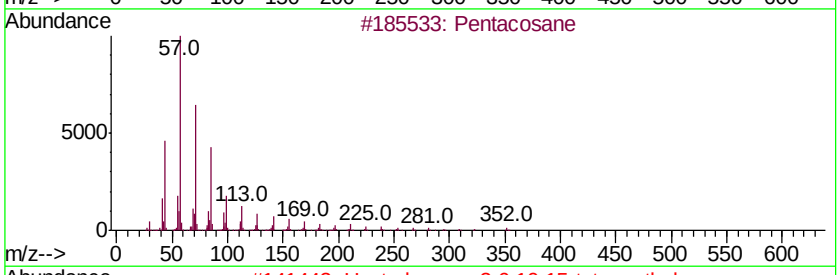
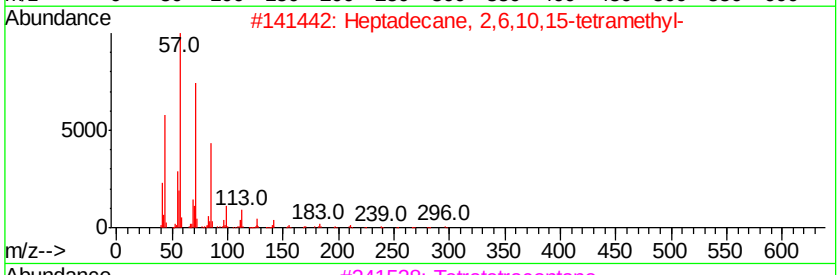
Peak Number 9 Pentacosane Concentration Rank 8

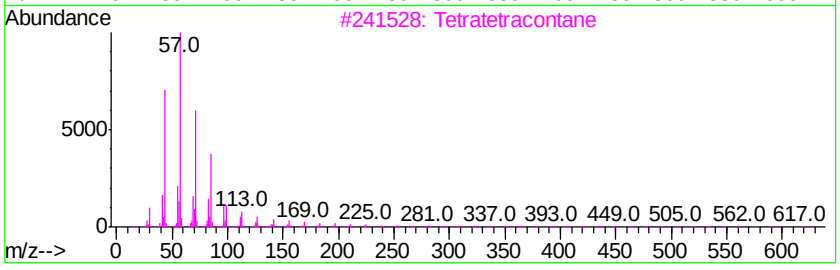
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	2.91 ng	164225	Chrysene-d12	14.22

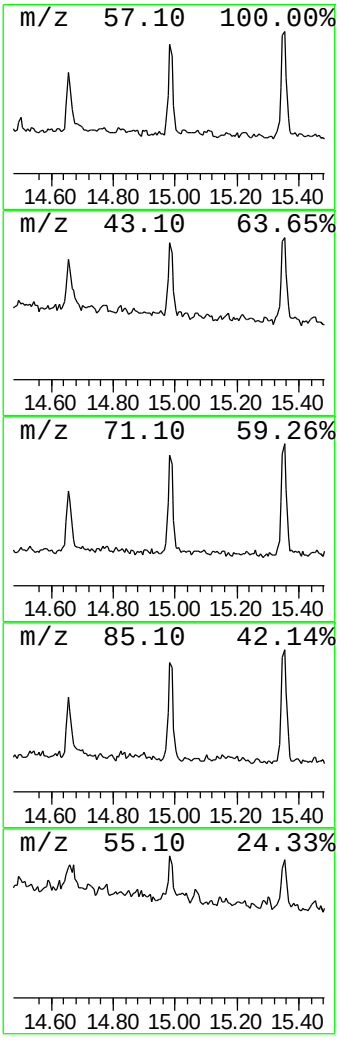
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	91
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	89
3	Tetratetracontane	619	C44H90	007098-22-8	87
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5	Heneicosane	296	C21H44	000629-94-7	87











Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081418\
Data File : BF108155.D
Acq On : 14 Aug 2018 19:56
Operator : JU/SJ
Sample : J4458-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-94

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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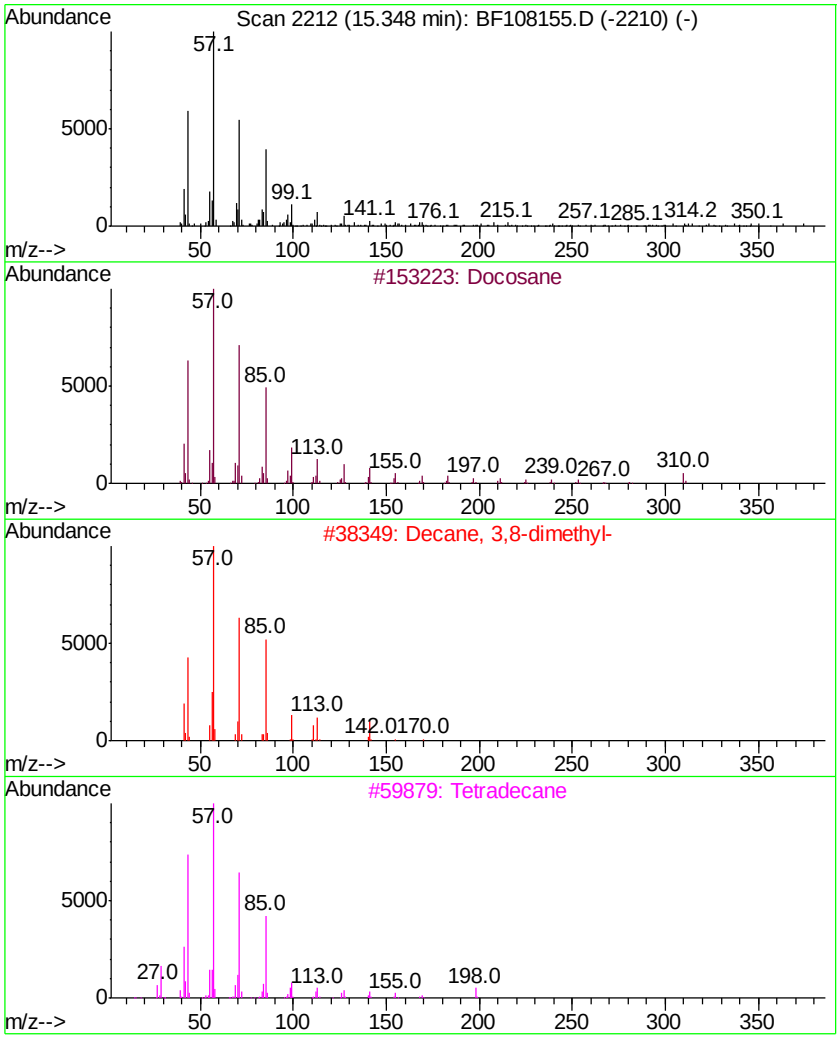
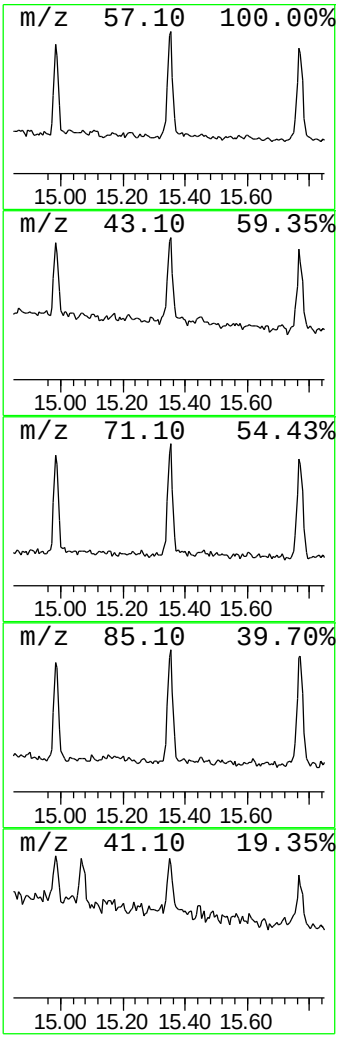
Peak Number 10 Docosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.35	4.44 ng	214595	Perylene-d12	15.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	93
2	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
3	Tetradecane	198	C14H30	000629-59-4	87
4	Heptadecane	240	C17H36	000629-78-7	87
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081418\
Data File : BF108155.D
Acq On : 14 Aug 2018 19:56
Operator : JU/SJ
Sample : J4458-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-94

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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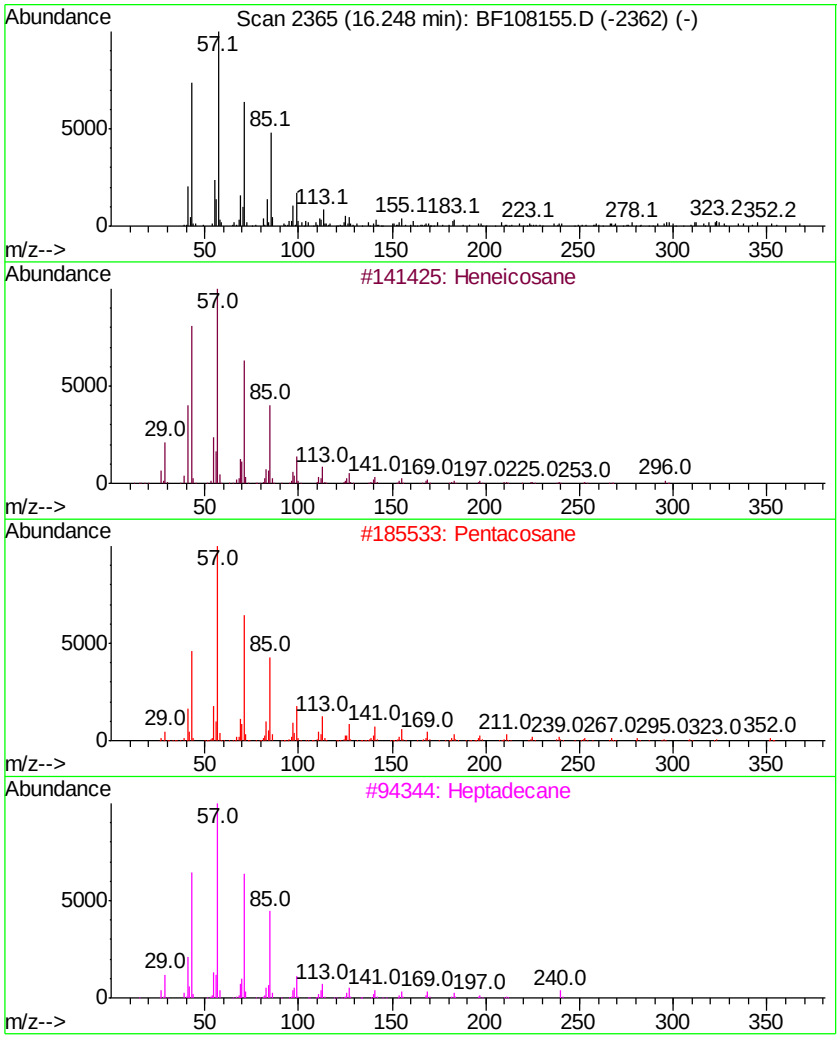
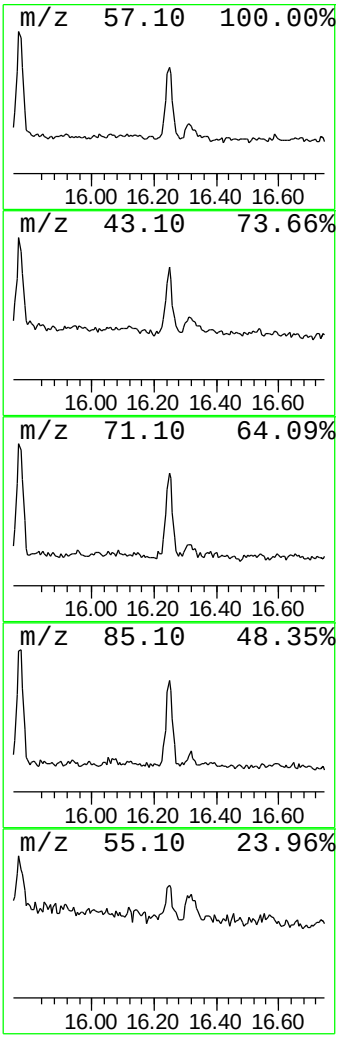
Peak Number 11 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.25	4.06 ng	196459	Perylene-d12	15.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	93
2	Pentacosane	352	C25H52	000629-99-2	93
3	Heptadecane	240	C17H36	000629-78-7	87
4	2-methyloctacosane	408	C29H60	1000376-72-8	86
5	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081418\
Data File : BF108155.D
Acq On : 14 Aug 2018 19:56
Operator : JU/SJ
Sample : J4458-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-94

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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...	2.37	39.0	ng	2175720	1	7.02	1115880	20.0
2-Pentanone, 4-hy...	5.25	2.1	ng	117773	1	7.02	1115880	20.0
unknown6.78	6.78	29.8	ng	1661210	1	7.02	1115880	20.0
Octacosane	10.95	2.4	ng	145120	4	11.56	1187910	20.0
n-Hexadecanoic acid	12.07	8.5	ng	505733	4	11.56	1187910	20.0
Octadecanoic acid	12.86	2.5	ng	146088	4	11.56	1187910	20.0
Trichloroacetic a...	14.03	11.8	ng	666018	5	14.22	1127730	20.0
Pentacosane	14.98	2.9	ng	164225	5	14.22	1127730	20.0
Docosane	15.35	4.4	ng	214595	6	15.78	966971	20.0
Heneicosane	16.25	4.1	ng	196459	6	15.78	966971	20.0