LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041018\
Data File : BF104412.D
Acq On : 10 Apr 2018 16:47
Operator : JU/SJ
Sample : J2303-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M11

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-BF040618.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	5.016	494	498	506	rVB	99775	118959	4.83%	0.532%
2	5.416	561	566	569	rBV	2326666	2393328	97.09%	10.709%
3	6.063	673	676	682	rVB	27984	32024	1.30%	0.143%
4	6.439	734	740	750	rVB	2339276	2395018	97.16%	10.717%
5	6.575	759	763	766	rBV	2642548	2444173	99.15%	10.937%
6	6.810	799	803	806	rVB	850436	726481	29.47%	3.251%
7	6.963	825	829	832	rBV	2247612	1893172	76.80%	8.471%
8	7.375	893	899	901	rBV	1472610	1481118	60.09%	6.628%
9	8.092	1017	1021	1024	rBV	1141617	922356	37.42%	4.127%
10	9.169	1199	1204	1207	rBV	2984871	2465010	100.00%	11.030%
11	9.557	1267	1270	1274	rBV	178953	149477	6.06%	0.669%
12	9.774	1304	1307	1310	rVB	76210	55151	2.24%	0.247%
13	9.845	1315	1319	1323	rVB2	977022	848935	34.44%	3.799%
14	10.145	1366	1370	1374	rBV2	51954	51516	2.09%	0.231%
15	10.274	1390	1392	1395	rVB	90383	65039	2.64%	0.291%
16	10.498	1424	1430	1432	rBV3	28009	35943	1.46%	0.161%
17	10.633	1447	1453	1457	rBV	1283886	1196604	48.54%	5.354%
18	10.751	1470	1473	1477	rBV	77604	78510	3.18%	0.351%
19	11.198	1546	1549	1552	rBV	36627	35559	1.44%	0.159%
20	11.333	1569	1572	1575	rBV	807245	697293	28.29%	3.120%
21	11.357	1575	1576	1580	rVB	62588	38717	1.57%	0.173%
22	11.863	1659	1662	1668	rVB2	66888	68074	2.76%	0.305%
23	12.551	1775	1779	1783	rBV	96708	91408	3.71%	0.409%
24	12.774	1814	1817	1820	rBV	81148	75339	3.06%	0.337%
25	12.921	1838	1842	1846	rBV	1963316	1896852	76.95%	8.488%
26	13.462	1931	1934	1936	rBV	120412	98543	4.00%	0.441%
27	13.815	1991	1994	1999	rBV	150118	157835	6.40%	0.706%
28	13.980	2017	2022	2025	rBV	853104	840609	34.10%	3.761%
29	14.004	2025	2026	2029	rVB	64672	37535	1.52%	0.168%
30	14.462	2101	2104	2108	rVB2	94864	98870	4.01%	0.442%
31	15.021	2196	2199	2206	rVB	49279	91652	3.72%	0.410%
32	15.104	2210	2213	2215	rBV	72547	76291	3.09%	0.341%
33	15.398	2259	2263	2267	rVB2	131315	169199	6.86%	0.757%
34	15.451	2267	2272	2275	rBV	442543	521201	21.14%	2.332%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041018\
Data File : BF104412.D
Acq On : 10 Apr 2018 16:47
Operator : JU/SJ
Sample : J2303-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M11

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-BF040618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 22347791

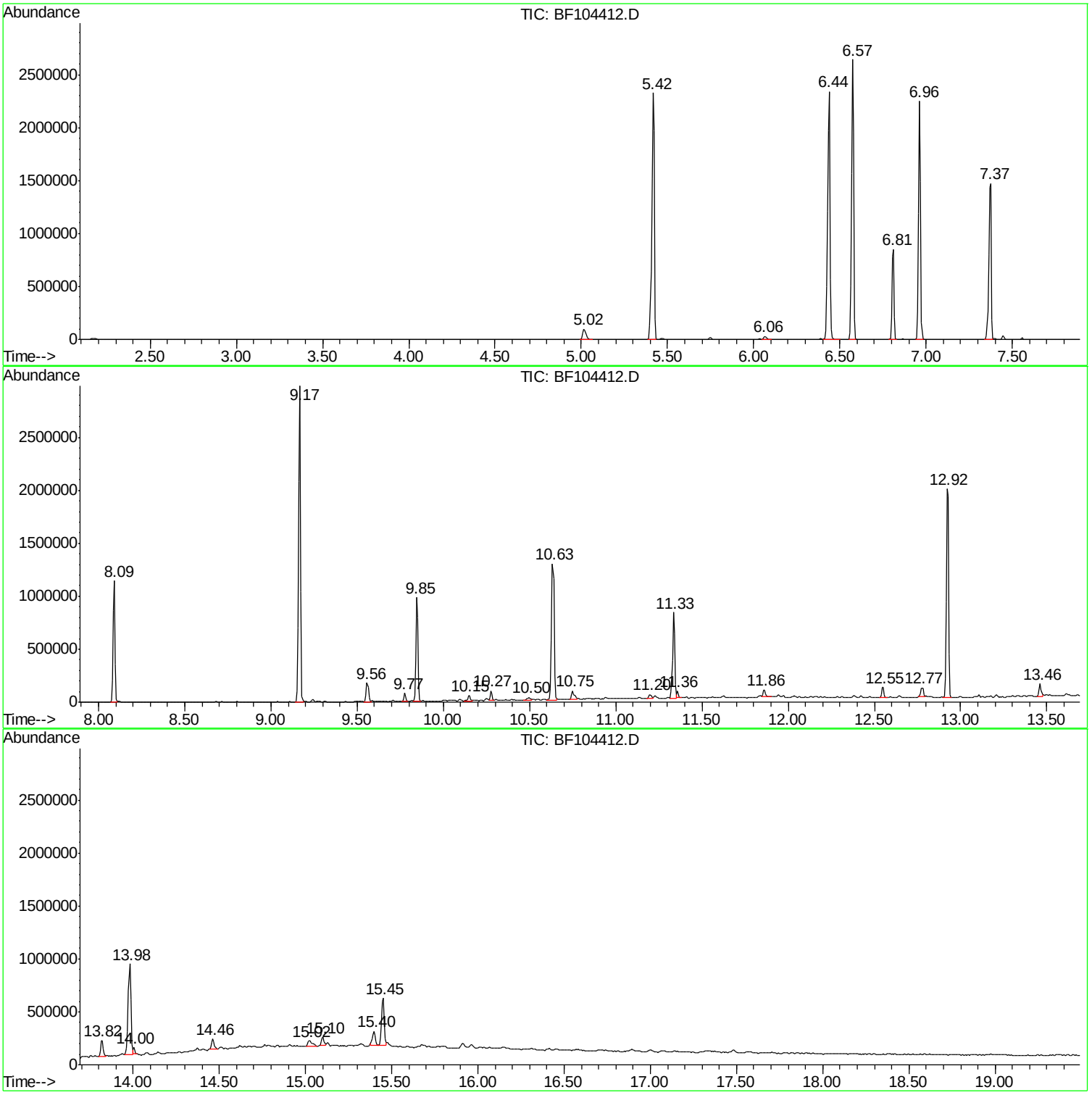
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041018\
Data File : BF104412.D
Acq On : 10 Apr 2018 16:47
Operator : JU/SJ
Sample : J2303-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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 F\DATA\BF041018\
Data File : BF104412.D
Acq On : 10 Apr 2018 16:47
Operator : JU/SJ
Sample : J2303-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

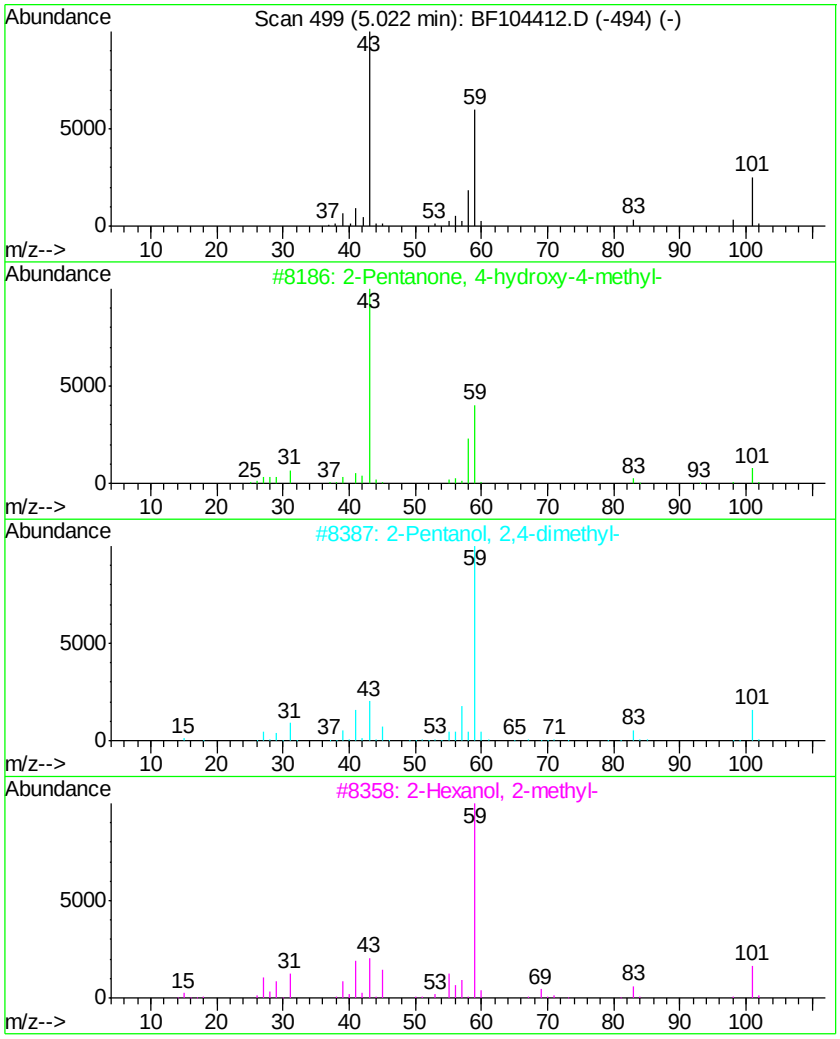
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

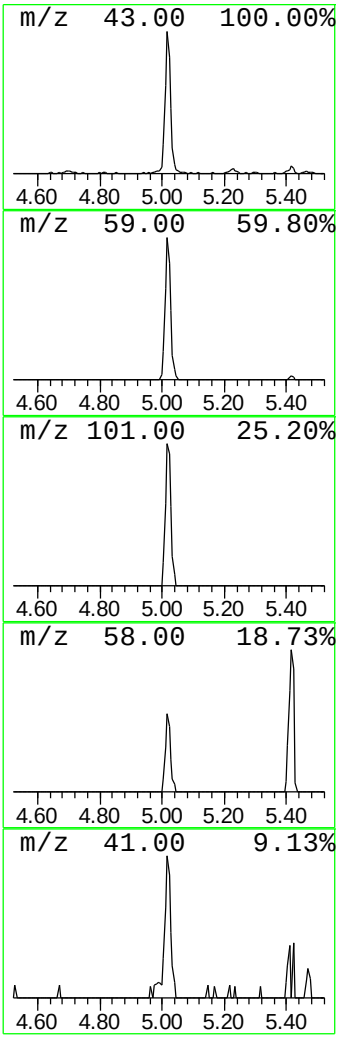
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	3.27 ng	118959	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	42
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041018\
Data File : BF104412.D
Acq On : 10 Apr 2018 16:47
Operator : JU/SJ
Sample : J2303-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

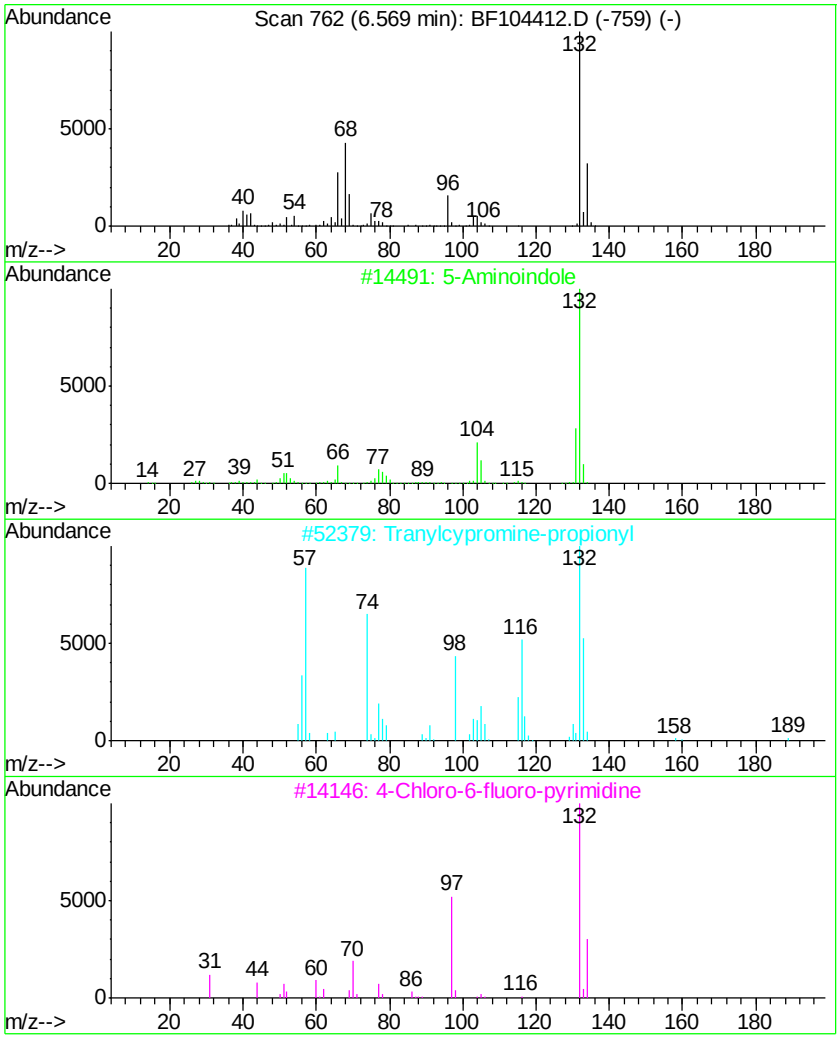
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

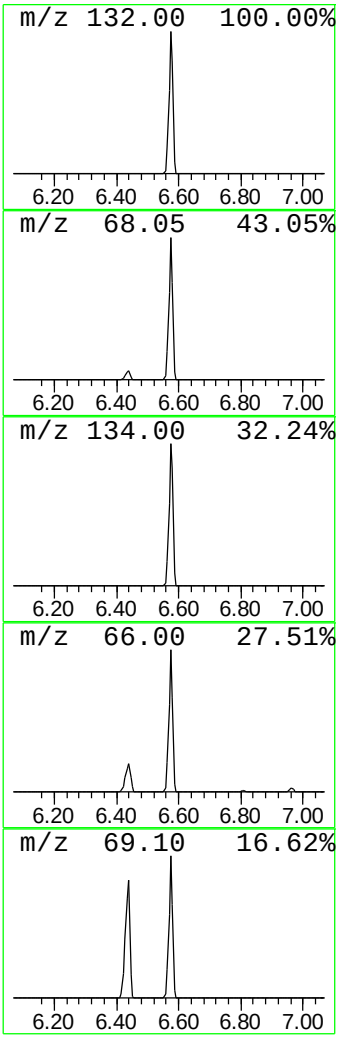
****

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	67.29 ng	2444170	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041018\
Data File : BF104412.D
Acq On : 10 Apr 2018 16:47
Operator : JU/SJ
Sample : J2303-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

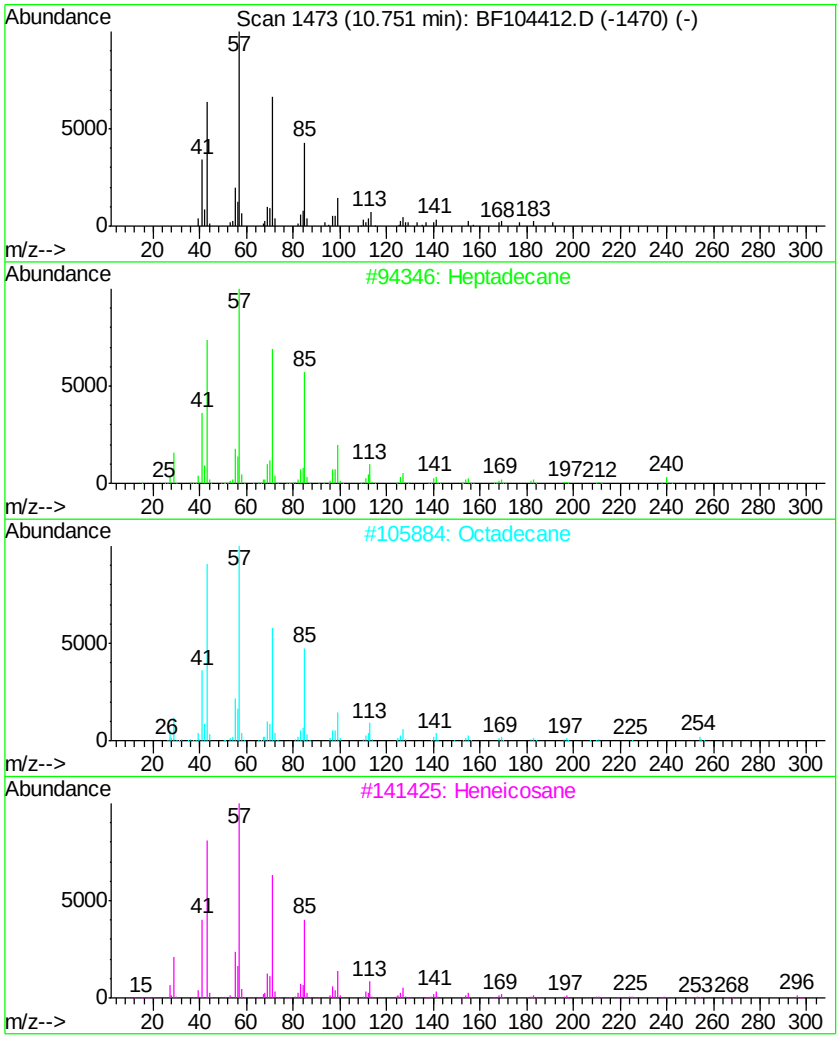
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

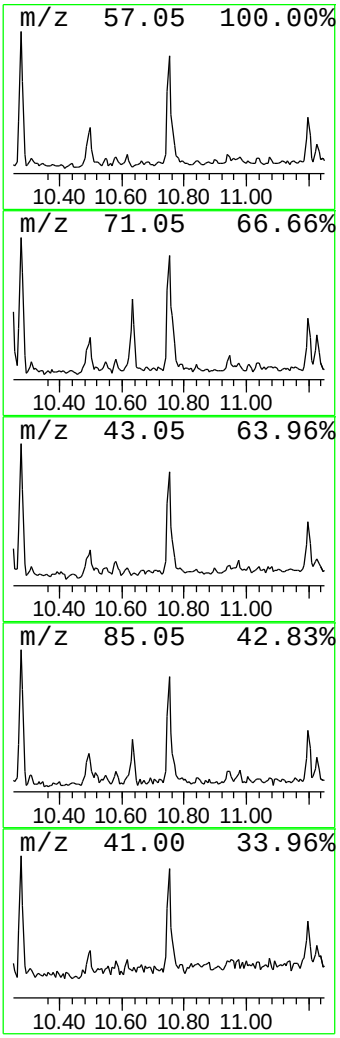
****

Peak Number 4 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	2.25 ng	78510	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Octadecane	254	C18H38	000593-45-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Tetradecane	198	C14H30	000629-59-4	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041018\
Data File : BF104412.D
Acq On : 10 Apr 2018 16:47
Operator : JU/SJ
Sample : J2303-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

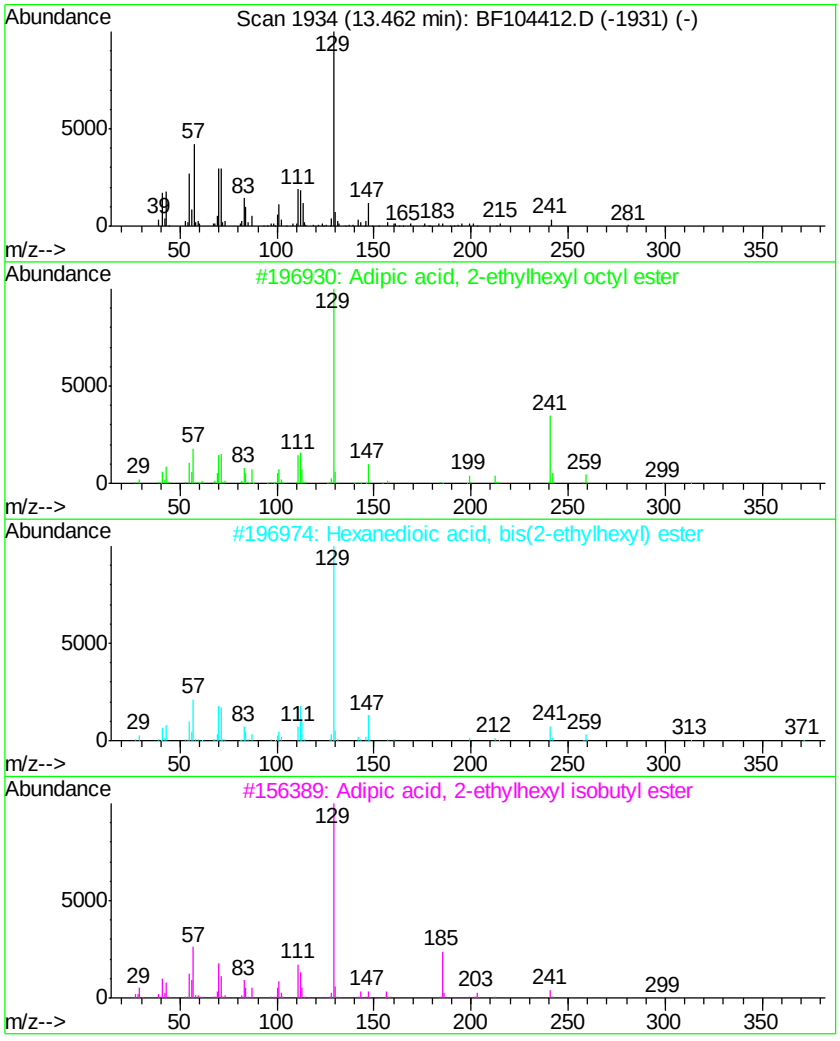
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

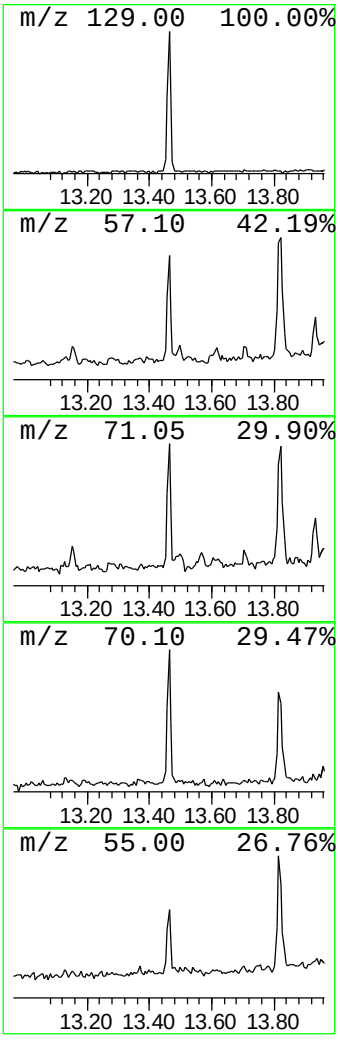
****

Peak Number 5 Adipic acid, 2-ethylhexyl o... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.46	2.34 ng	98543	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	91
2	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	90
3	Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1000324-48-0	72
4	Adipic acid, 2-ethylhexyl pentyl...	328	C19H36O4	1000324-48-2	64
5	Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	58





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041018\
Data File : BF104412.D
Acq On : 10 Apr 2018 16:47
Operator : JU/SJ
Sample : J2303-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

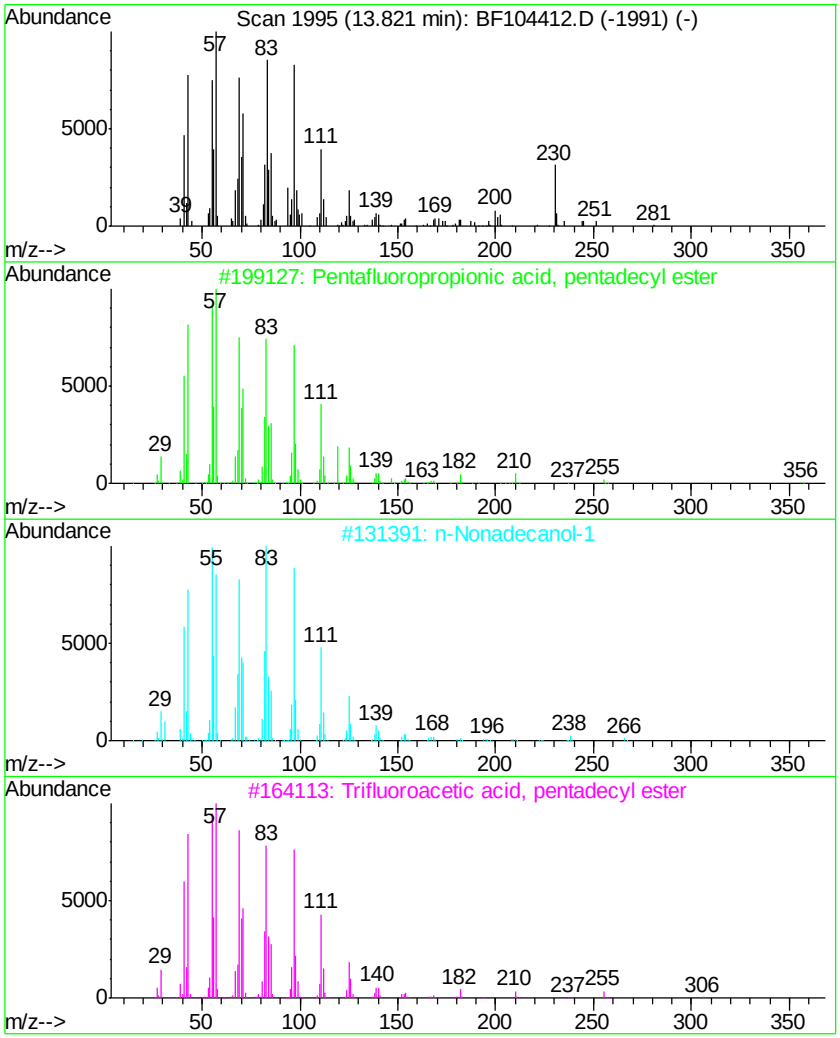
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

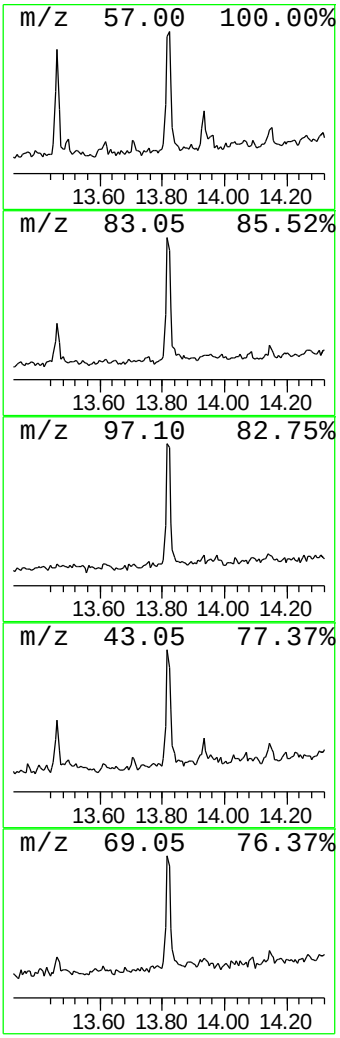
****

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	3.76 ng	157835	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	93





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041018\
Data File : BF104412.D
Acq On : 10 Apr 2018 16:47
Operator : JU/SJ
Sample : J2303-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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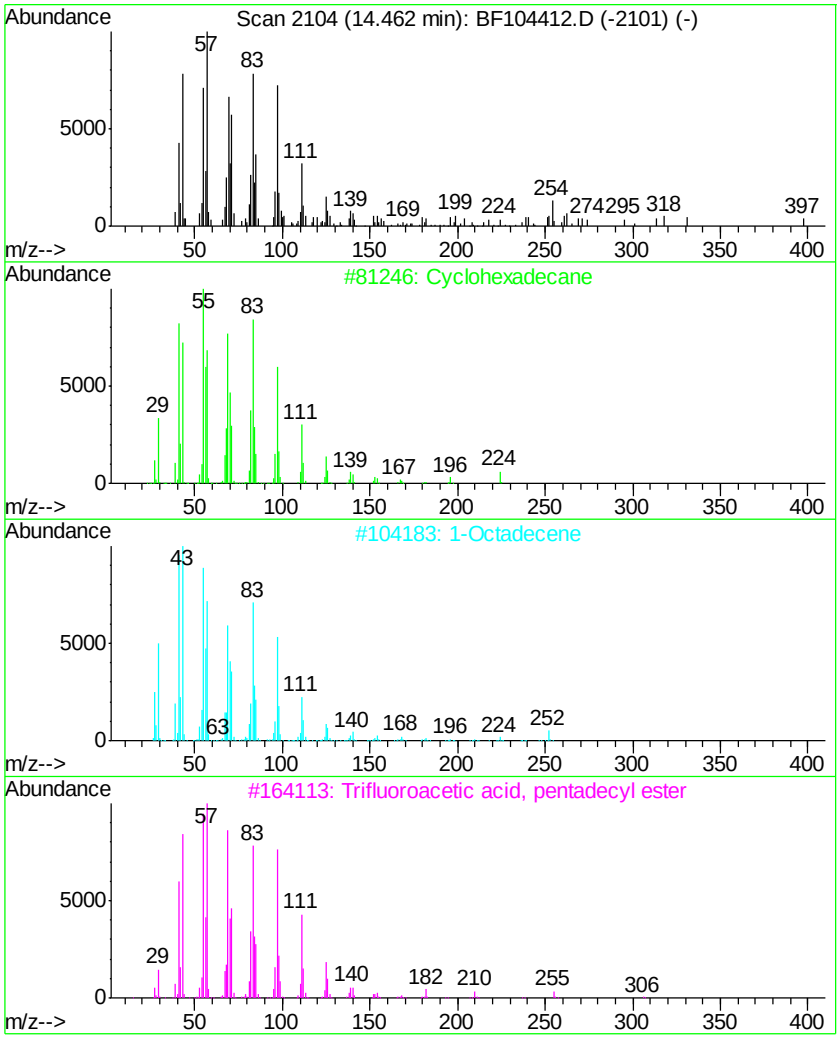
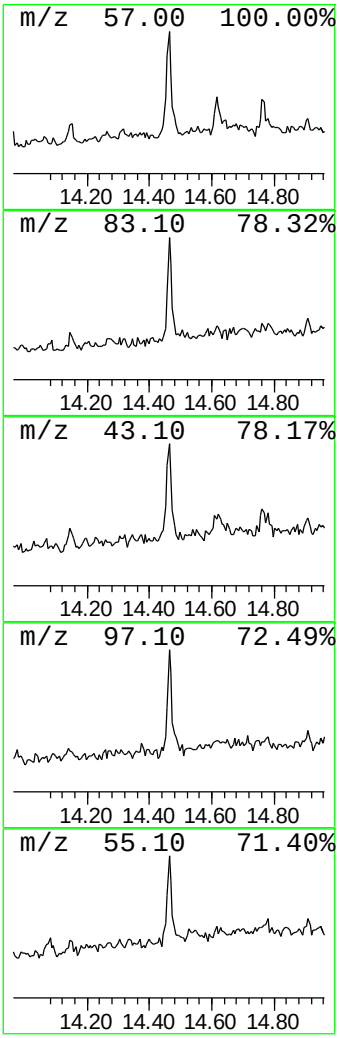
Peak Number 7 Cyclohexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.46	2.35 ng	98870	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	94
2	1-Octadecene	252	C18H36	000112-88-9	93
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041018\
Data File : BF104412.D
Acq On : 10 Apr 2018 16:47
Operator : JU/SJ
Sample : J2303-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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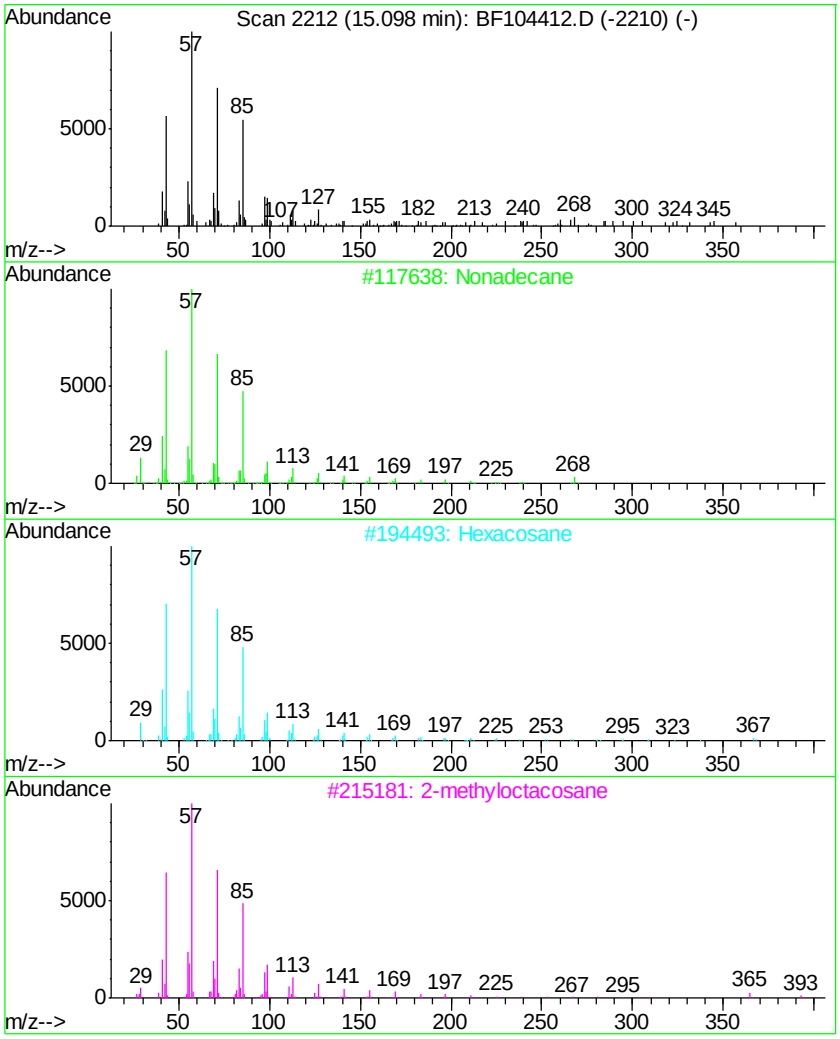
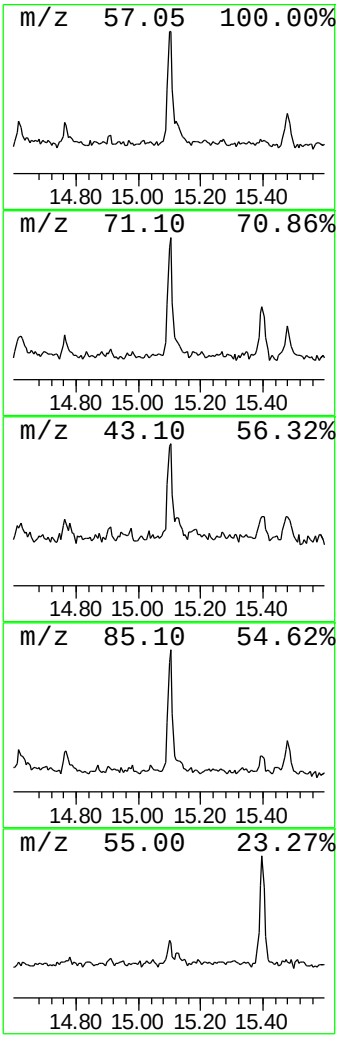
Peak Number 8 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.10	2.93 ng	76291	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	93
2	Hexacosane	366	C26H54	000630-01-3	90
3	2-methyloctacosane	408	C29H60	1000376-72-8	90
4	Hexadecane	226	C16H34	000544-76-3	86
5	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	83





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041018\
Data File : BF104412.D
Acq On : 10 Apr 2018 16:47
Operator : JU/SJ
Sample : J2303-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

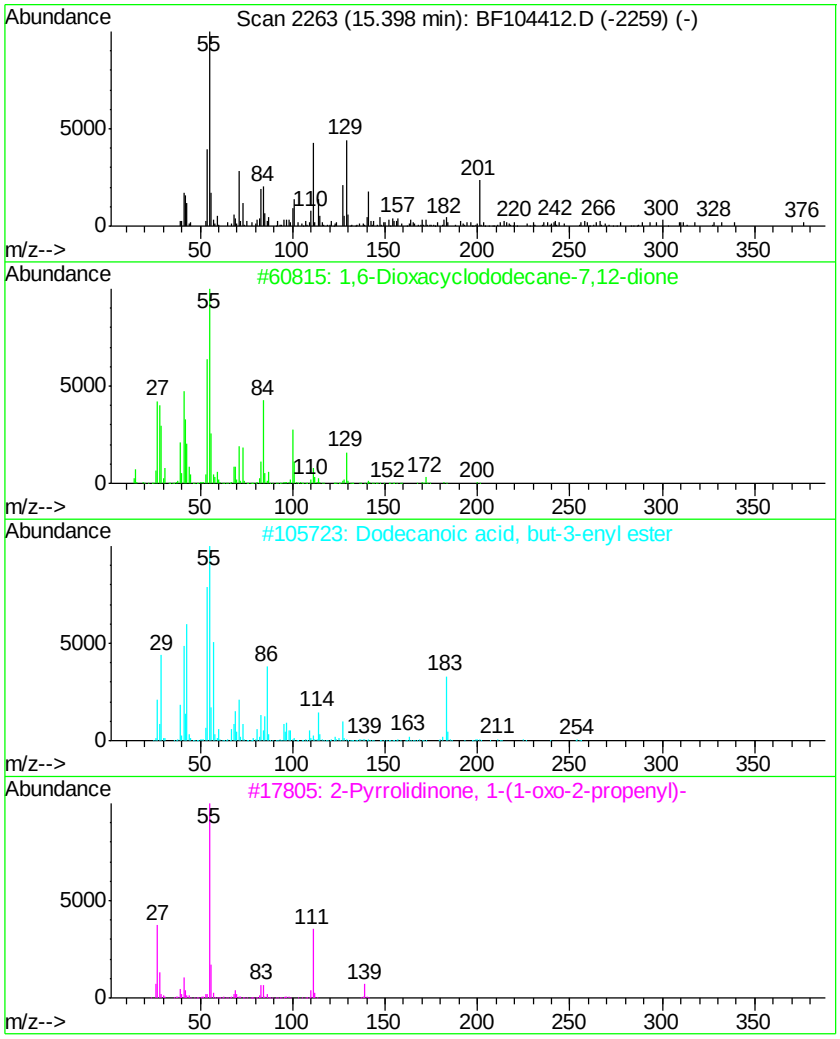
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

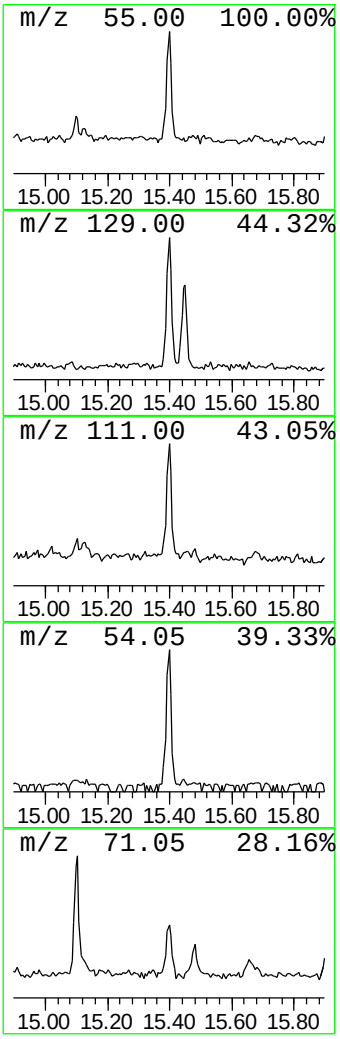
****

Peak Number 9 unknown15.40 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.40	6.49 ng	169199	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6-Dioxacyclododecane-7,12-dione	200	C10H16O4	000777-95-7	10
2	Dodecanoic acid, but-3-enyl ester	254	C16H30O2	1000159-94-4	10
3	2-Pyrrolidinone, 1-(1-oxo-2-prop...	139	C7H9NO2	002043-26-7	9
4	Butanedioic acid, 2-methyl-3-oxo...	202	C9H14O5	000759-65-9	9
5	1H-Tetrazole-5-acetic acid, ethy...	156	C5H8N4O2	013616-37-0	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041018\
Data File : BF104412.D
Acq On : 10 Apr 2018 16:47
Operator : JU/SJ
Sample : J2303-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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...	5.02	3.3	ng	118959	1	6.81	726481	20.0
unknown6.57	6.57	67.3	ng	2444170	1	6.81	726481	20.0
Heptadecane	10.75	2.3	ng	78510	4	11.33	697293	20.0
Adipic acid, 2-et...	13.46	2.3	ng	98543	5	13.98	840609	20.0
Pentafluoropropio...	13.82	3.8	ng	157835	5	13.98	840609	20.0
Cyclohexadecane	14.46	2.4	ng	98870	5	13.98	840609	20.0
Nonadecane	15.10	2.9	ng	76291	6	15.45	521201	20.0
unknown15.40	15.40	6.5	ng	169199	6	15.45	521201	20.0