LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062216\
Data File : BF088264.D
Acq On : 22 Jun 2016 22:14
Operator : UM/SJ
Sample : H3676-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCHC-011

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-BF060716.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	1.724	11	12	47	rVB	1295205	2723228	100.00%	12.464%
2	4.730	274	275	288	rBV	192070	388291	14.26%	1.777%
3	5.187	313	315	318	rBV	1665822	1815446	66.67%	8.309%
4	6.262	407	409	416	rBV	1630176	1907789	70.06%	8.732%
5	6.376	416	419	421	rBV	1897262	2195231	80.61%	10.047%
6	6.605	437	439	441	rBV	398817	420411	15.44%	1.924%
7	6.753	450	452	455	rBV	1561783	1614089	59.27%	7.387%
8	7.176	487	489	491	rBV	1307003	1337415	49.11%	6.121%
9	7.885	549	551	554	rBV	617286	602878	22.14%	2.759%
10	8.970	643	646	648	rBV	2482835	2394352	87.92%	10.959%
11	9.371	679	681	683	rBV	296621	253090	9.29%	1.158%
12	9.405	683	684	690	rVB2	144955	155938	5.73%	0.714%
13	9.588	698	700	702	rBV	26637	29662	1.09%	0.136%
14	9.633	702	704	707	rVV	684717	647399	23.77%	2.963%
15	10.079	741	743	745	rBV	45556	38186	1.40%	0.175%
16	10.422	771	773	776	rBV	1168147	1197700	43.98%	5.482%
17	10.548	782	784	788	rVB	51427	68934	2.53%	0.315%
18	10.994	822	823	825	rBV	37026	36817	1.35%	0.169%
19	11.108	832	833	836	rBV	442641	586140	21.52%	2.683%
20	12.331	937	940	942	rBV	32479	49359	1.81%	0.226%
21	12.548	956	959	961	rBV	32580	43880	1.61%	0.201%
22	12.697	969	972	974	rBV	1797463	1724418	63.32%	7.892%
23	13.611	1049	1052	1057	rBV	52779	130267	4.78%	0.596%
24	13.737	1061	1063	1066	rBV	326529	486498	17.86%	2.227%
25	13.920	1077	1079	1081	rBV	36512	42794	1.57%	0.196%
26	14.228	1104	1106	1107	rBV	27521	31925	1.17%	0.146%
27	14.514	1129	1131	1135	rBV3	24791	55445	2.04%	0.254%
28	14.640	1140	1142	1145	rVV4	24900	37794	1.39%	0.173%
29	14.811	1155	1157	1158	rVB	43777	41992	1.54%	0.192%
30	15.108	1181	1183	1189	rVB	371815	448962	16.49%	2.055%
31	15.497	1214	1217	1223	rBV3	52943	124690	4.58%	0.571%
32	15.668	1230	1232	1239	rVB2	53495	126086	4.63%	0.577%
33	16.023	1261	1263	1269	rVB2	30563	58966	2.17%	0.270%
34	16.503	1303	1305	1308	rVB2	22659	33181	1.22%	0.152%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062216\
Data File : BF088264.D
Acq On : 22 Jun 2016 22:14
Operator : UM/SJ
Sample : H3676-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCHC-011

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-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

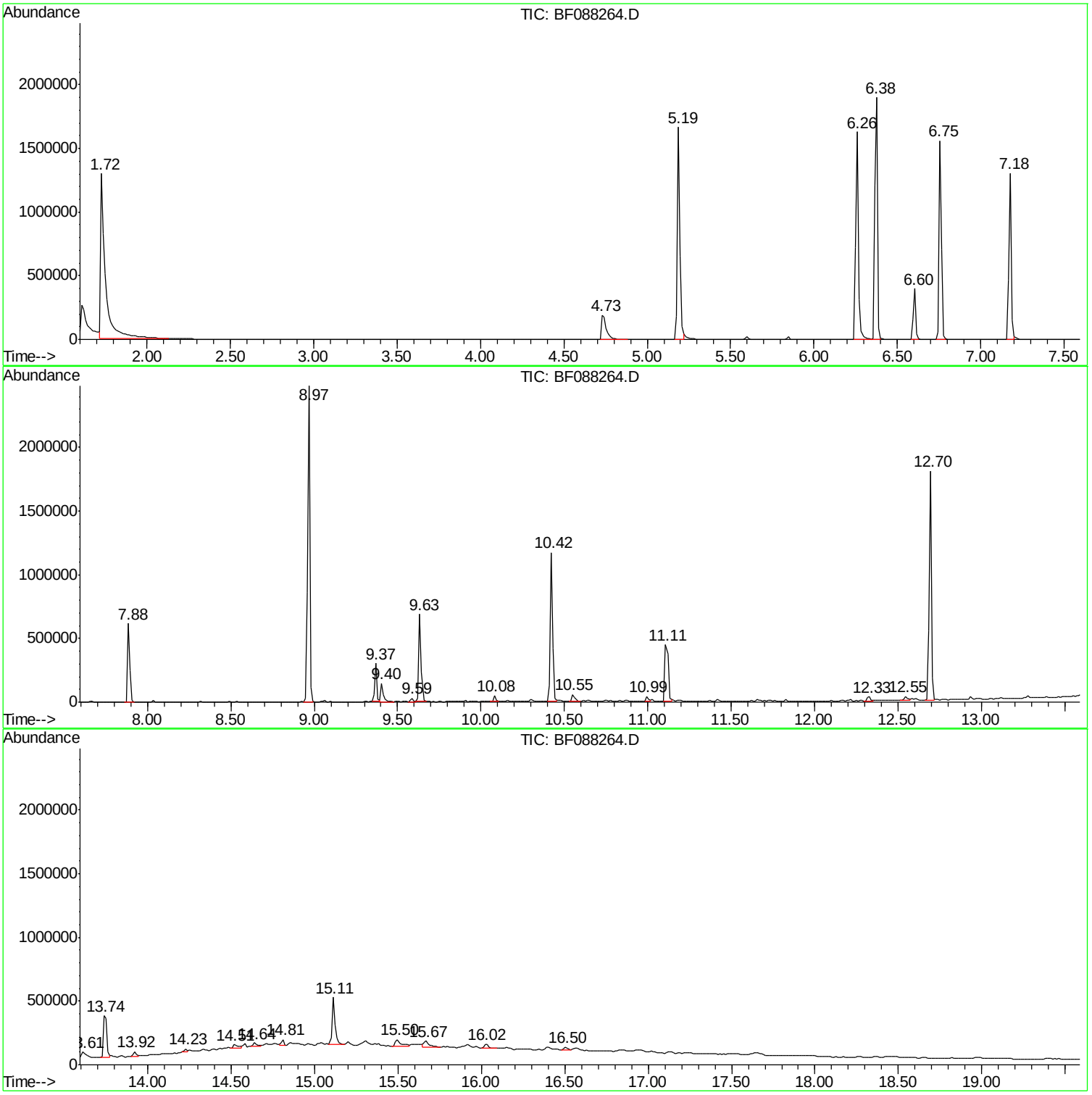
Sum of corrected areas: 21849253

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062216\
Data File : BF088264.D
Acq On : 22 Jun 2016 22:14
Operator : UM/SJ
Sample : H3676-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NCHC-011

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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\BF062216\
Data File : BF088264.D
Acq On : 22 Jun 2016 22:14
Operator : UM/SJ
Sample : H3676-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCHC-011

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

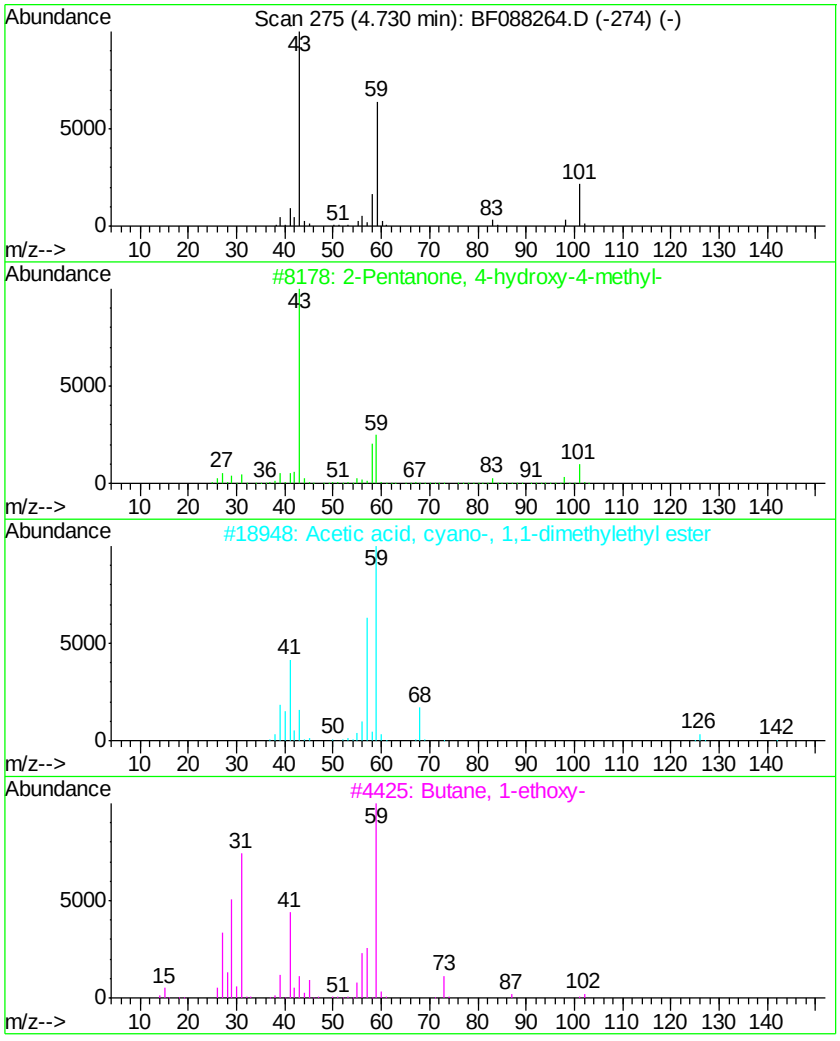
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

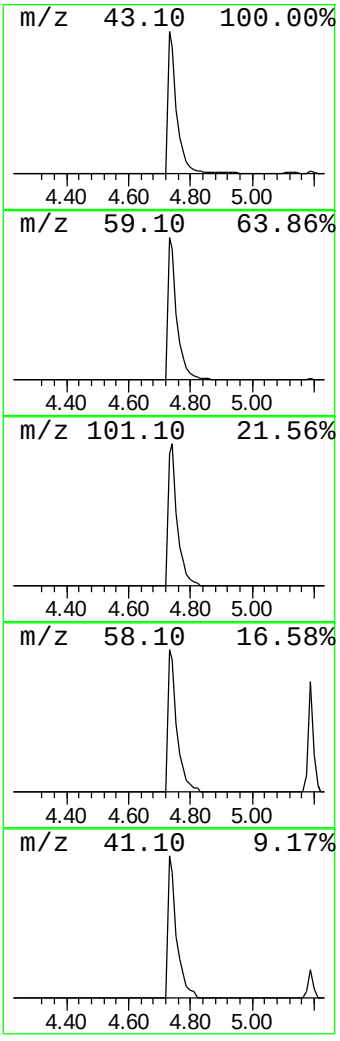
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.73	18.47 ng	388291	1,4-Dichlorobenzene-d4	6.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062216\
Data File : BF088264.D
Acq On : 22 Jun 2016 22:14
Operator : UM/SJ
Sample : H3676-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCHC-011

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

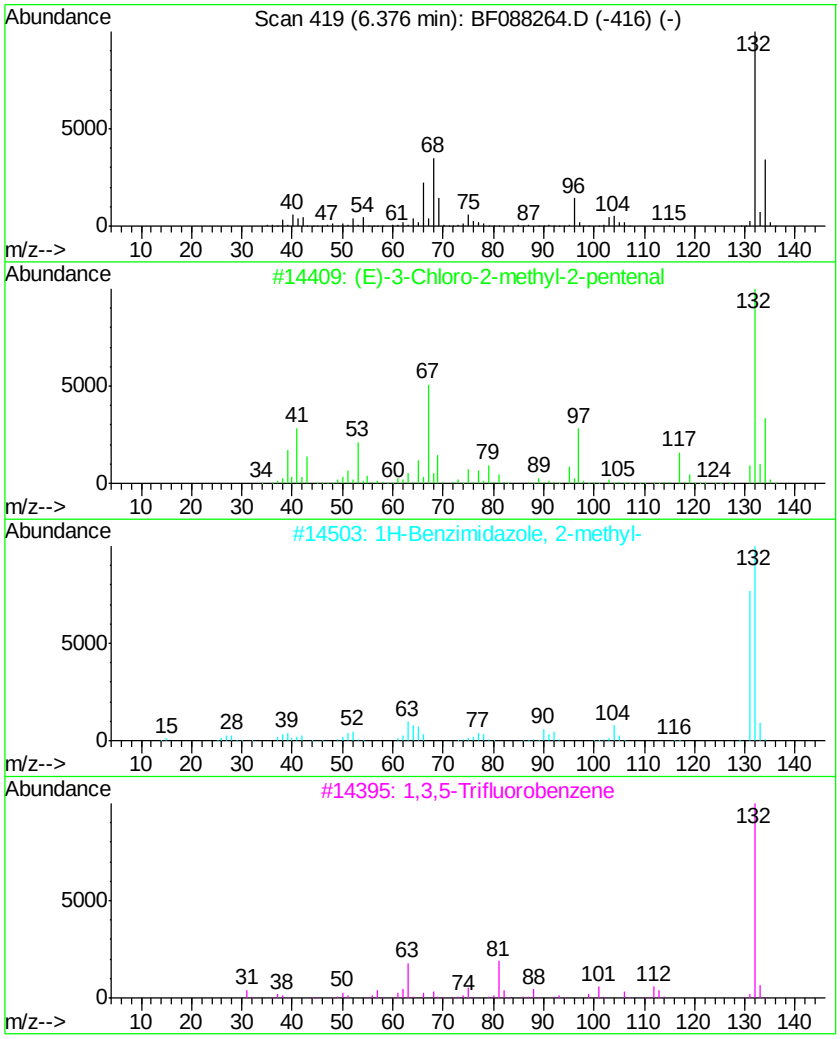
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

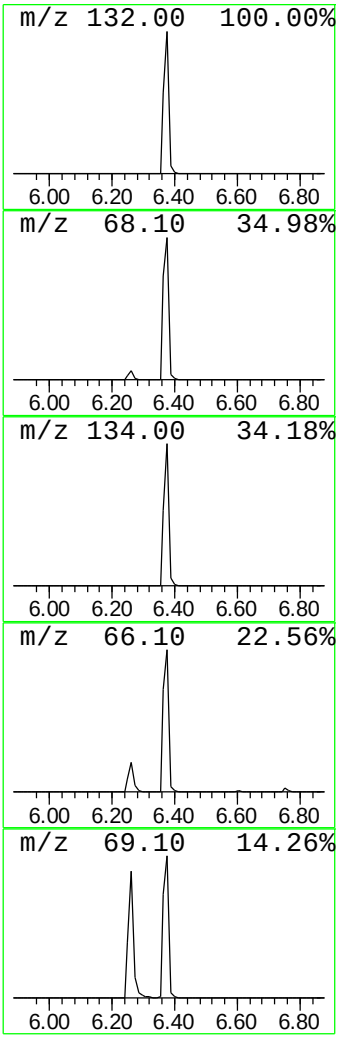
****

Peak Number 3 unknown6.38 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.38	104.43 ng	2195230	1,4-Dichlorobenzene-d4	6.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062216\
Data File : BF088264.D
Acq On : 22 Jun 2016 22:14
Operator : UM/SJ
Sample : H3676-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCHC-011

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

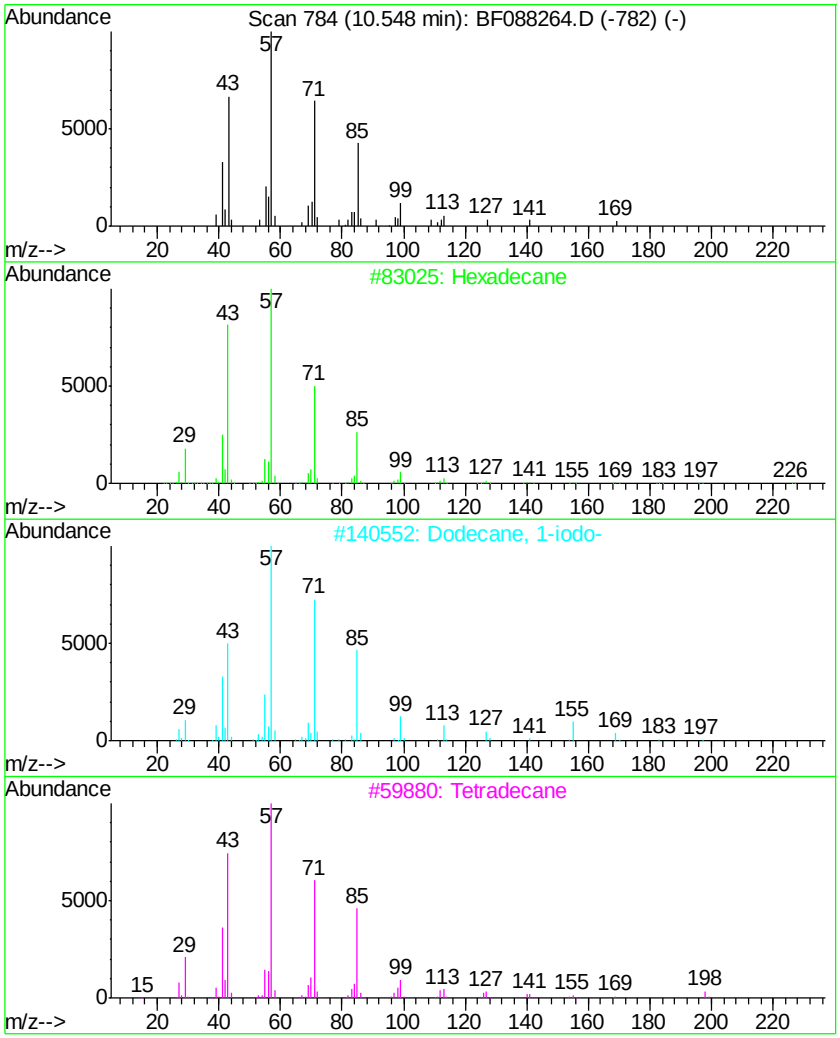
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

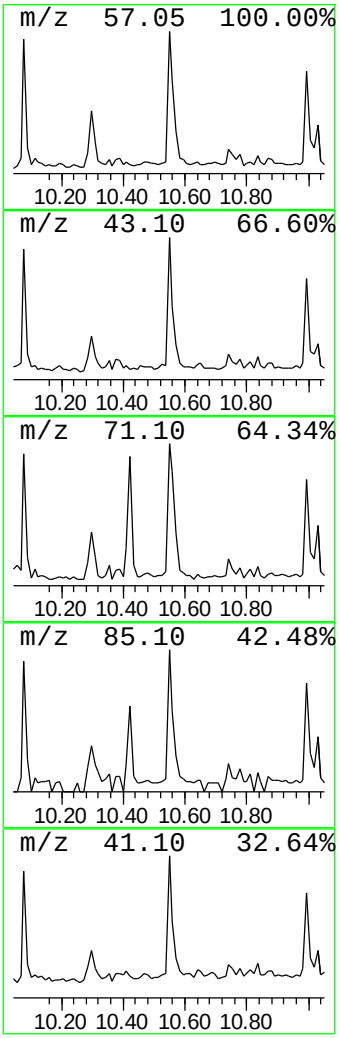
****

Peak Number 5 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.55	2.35 ng	68934	Phenanthrene-d10	11.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
3	Tetradecane	198	C14H30	000629-59-4	86
4	Eicosane	282	C20H42	000112-95-8	86
5	Pentadecane	212	C15H32	000629-62-9	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062216\
Data File : BF088264.D
Acq On : 22 Jun 2016 22:14
Operator : UM/SJ
Sample : H3676-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCHC-011

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

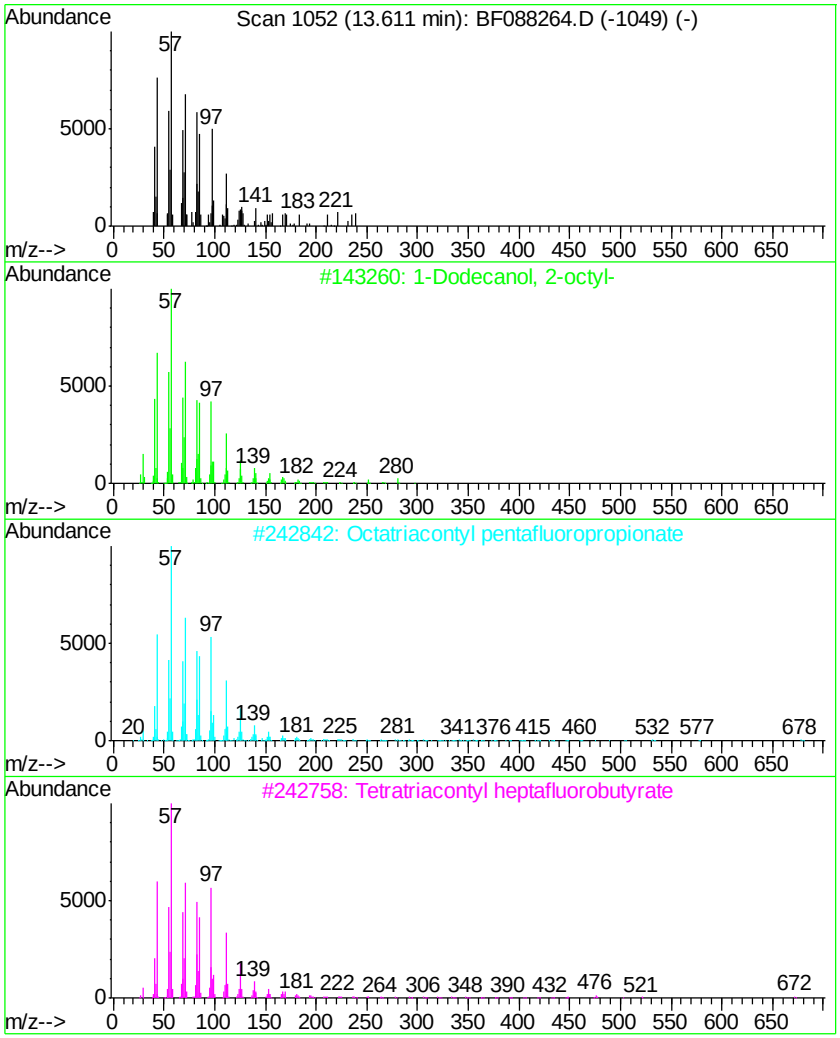
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

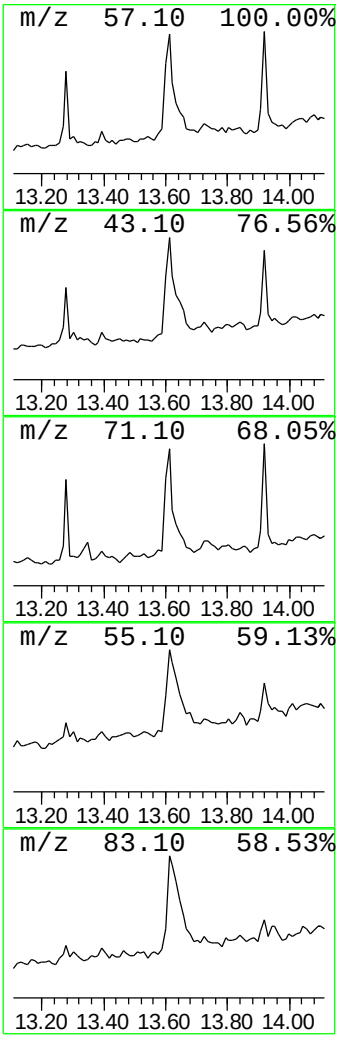
****

Peak Number 6 1-Dodecanol, 2-octyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.61	5.36 ng	130267	Chrysene-d12	13.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	90
2	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	87
3	Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	83
4	Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	83
5	Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	83





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062216\
Data File : BF088264.D
Acq On : 22 Jun 2016 22:14
Operator : UM/SJ
Sample : H3676-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCHC-011

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

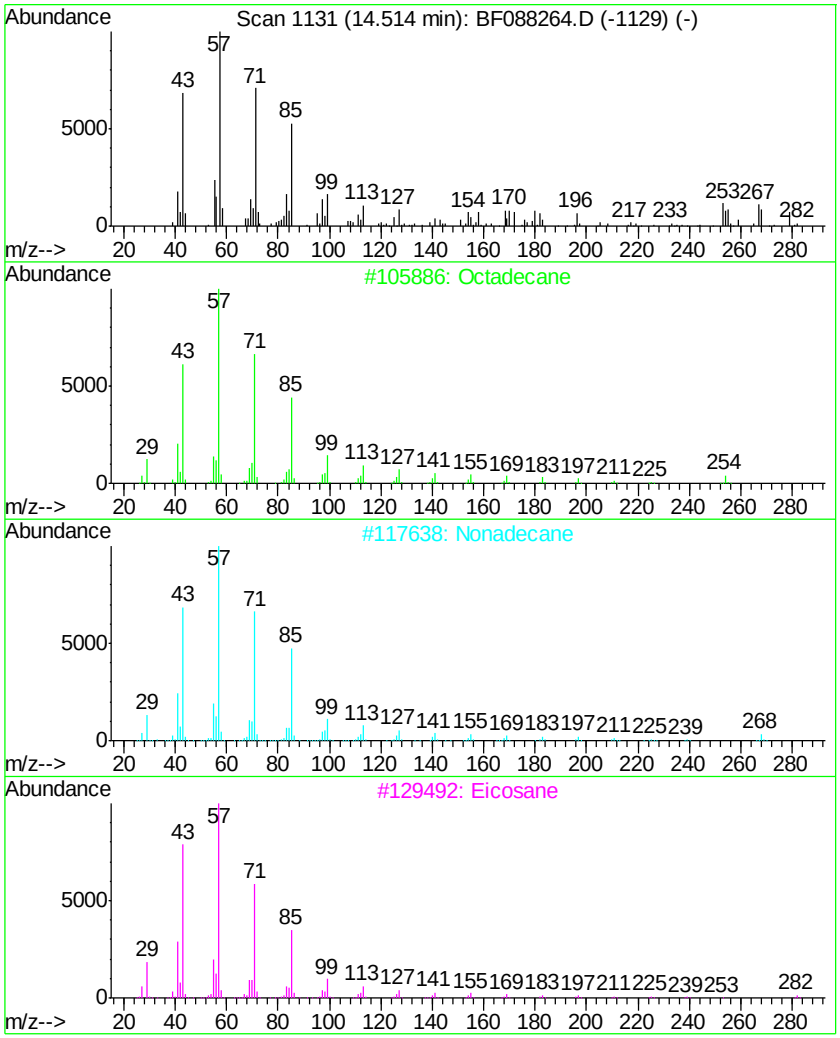
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

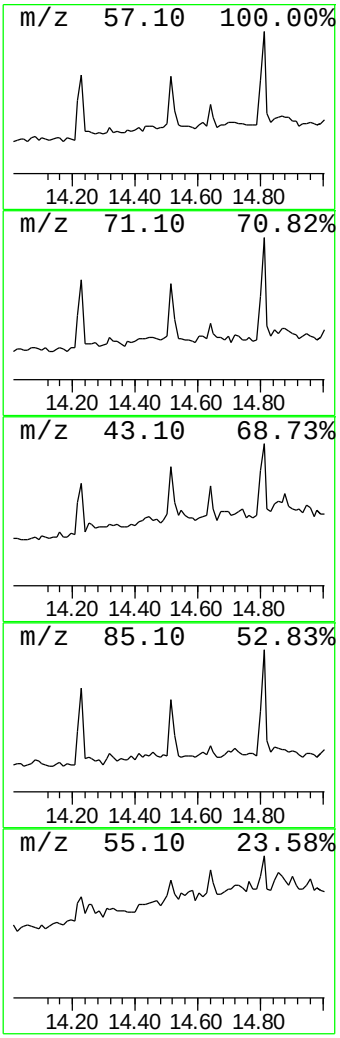
****

Peak Number 7 Octadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.51	2.47 ng	55445	Perylene-d12	15.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	91
2	Nonadecane	268	C19H40	000629-92-5	83
3	Eicosane	282	C20H42	000112-95-8	78
4	Hexacosane	366	C26H54	000630-01-3	60
5	Tetracosane	338	C24H50	000646-31-1	53





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062216\
Data File : BF088264.D
Acq On : 22 Jun 2016 22:14
Operator : UM/SJ
Sample : H3676-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCHC-011

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

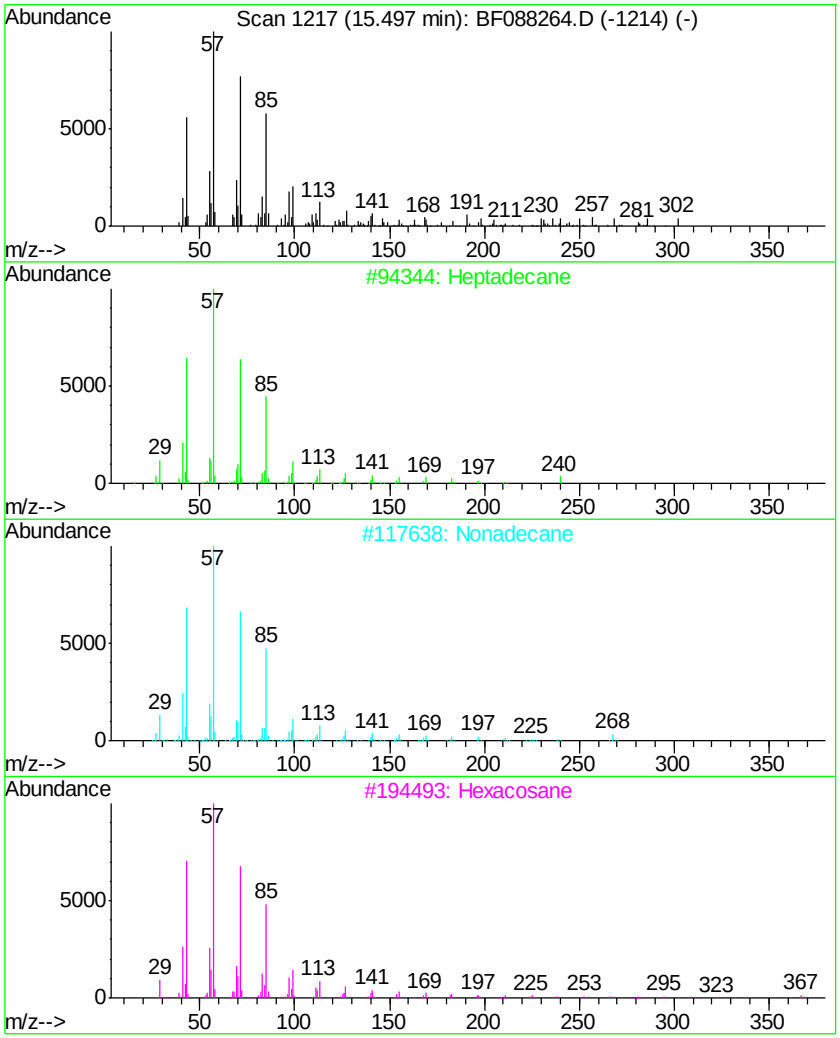
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

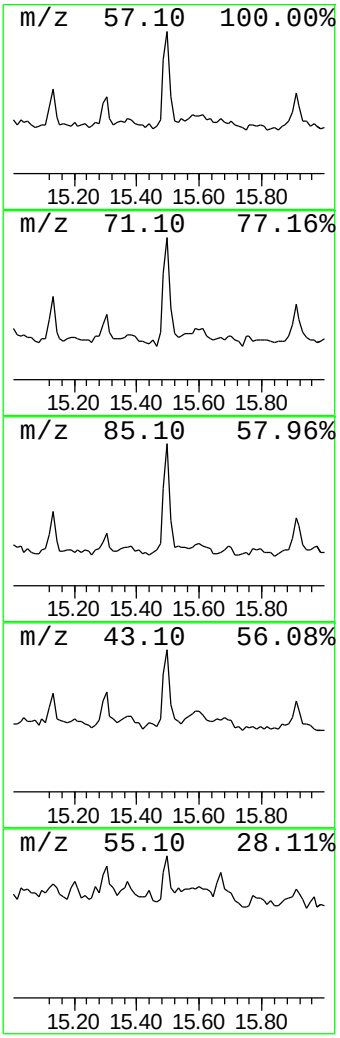
****

Peak Number 8 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.50	5.55 ng	124690	Perylene-d12	15.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	96
2	Nonadecane	268	C19H40	000629-92-5	96
3	Hexacosane	366	C26H54	000630-01-3	81
4	Heneicosane	296	C21H44	000629-94-7	81
5	2-methyloctacosane	408	C29H60	1000376-72-8	74





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062216\
Data File : BF088264.D
Acq On : 22 Jun 2016 22:14
Operator : UM/SJ
Sample : H3676-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCHC-011

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

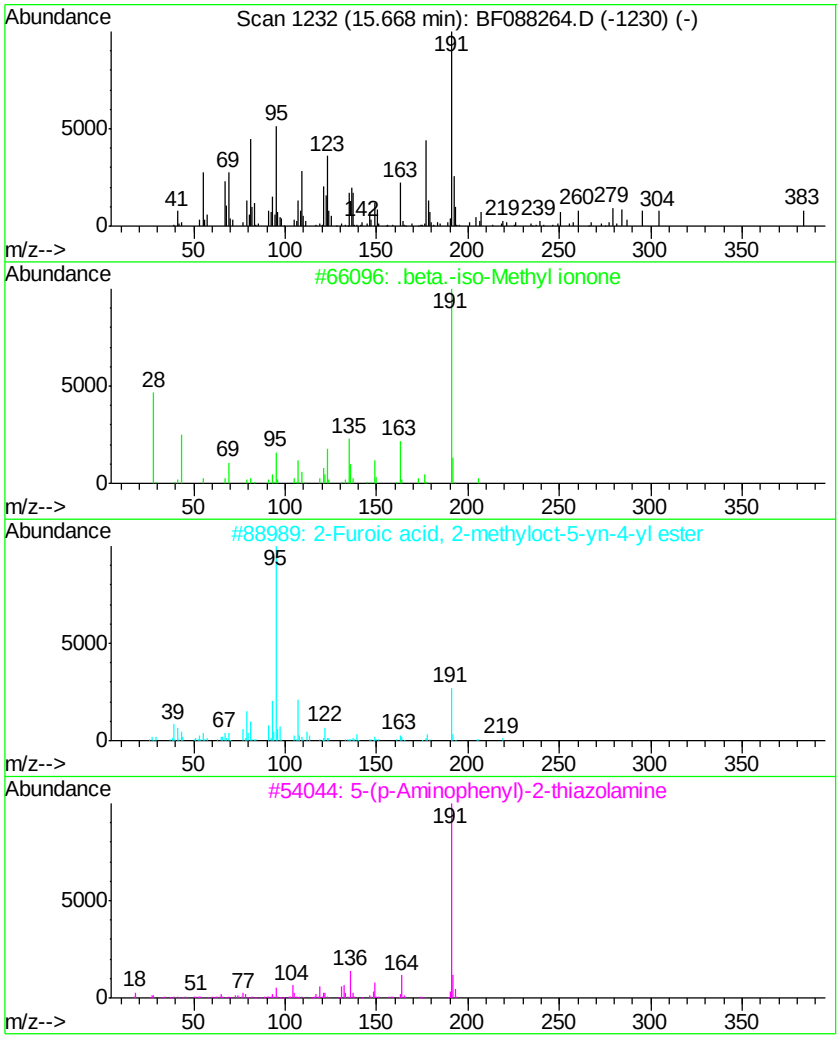
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

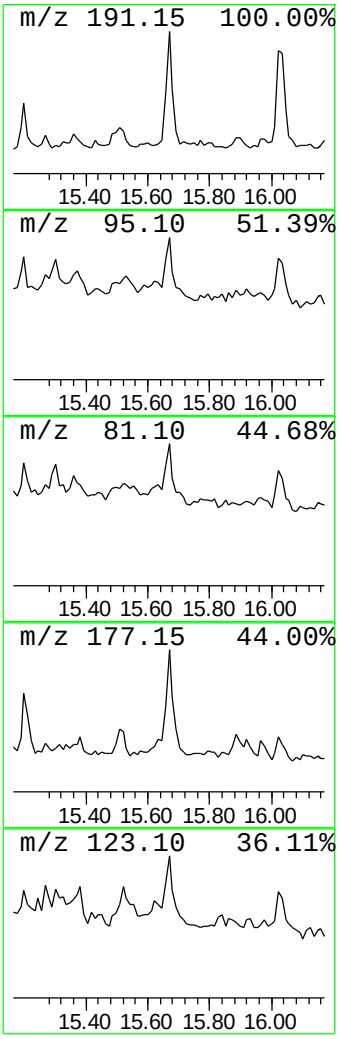
****

Peak Number 9 unknown15.67 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.67	5.62 ng	126086	Perylene-d12	15.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	43
2	2-Furoic acid, 2-methyloct-5-yn-...	234	C14H18O3	1000299-23-7	32
3	5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	27
4	Ethyl (1R,4S)-1,7,7-trimethylbic...	226	C13H22O3	1000373-77-2	25
5	2-Imino-3-phenyl-4-thiazolidinone	192	C9H8N2OS	006966-55-8	22





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062216\
Data File : BF088264.D
Acq On : 22 Jun 2016 22:14
Operator : UM/SJ
Sample : H3676-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCHC-011

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

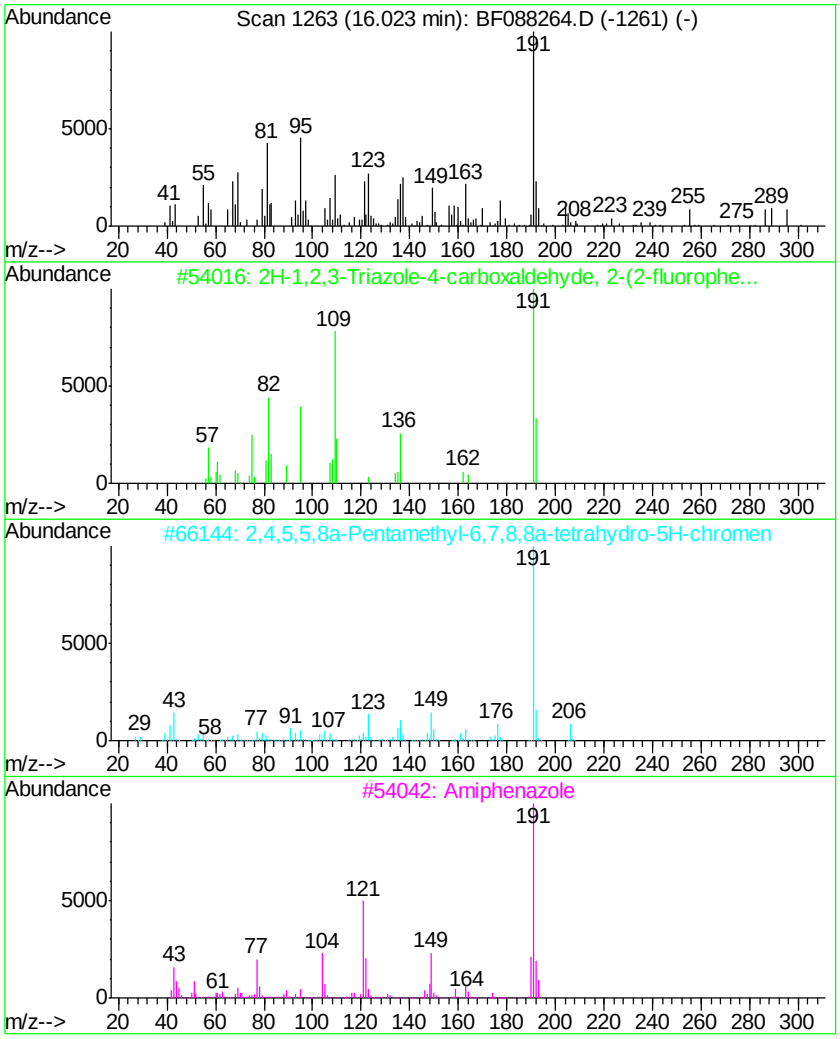
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

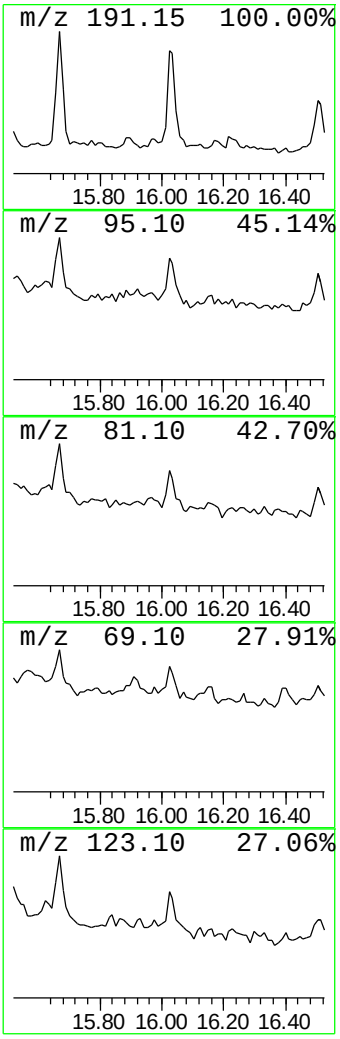
****

Peak Number 10 unknown16.02 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	2.63 ng	58966	Perylene-d12	15.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	43
2	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	38
3	Amiphenazole	191	C9H9N3S	000490-55-1	38
4	4-Fluoro-3-trifluoromethylbenzoi...	418	C23H34F4O2	1000338-69-0	27
5	2-Fluoro-6-trifluoromethylbenzoi...	278	C13H14F4O2	1000357-30-5	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062216\
Data File : BF088264.D
Acq On : 22 Jun 2016 22:14
Operator : UM/SJ
Sample : H3676-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCHC-011

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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...	4.73	18.5	ng	388291	1	6.60	420411	20.0
unknown6.38	6.38	104.4	ng	2195230	1	6.60	420411	20.0
Hexadecane	10.55	2.4	ng	68934	4	11.11	586140	20.0
1-Dodecanol, 2-oc...	13.61	5.4	ng	130267	5	13.75	486498	20.0
Octadecane	14.51	2.5	ng	55445	6	15.11	448962	20.0
Heptadecane	15.50	5.5	ng	124690	6	15.11	448962	20.0
unknown15.67	15.67	5.6	ng	126086	6	15.11	448962	20.0
unknown16.02	16.02	2.6	ng	58966	6	15.11	448962	20.0