LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121316\
Data File : BF091549.D
Acq On : 13 Dec 2016 13:04
Operator : UM/SJ
Sample : H5940-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS06-0-2IN

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-BF120916.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	5.001	252	255	262	rBV	2441616	3549948	37.90%	4.196%
2	5.424	289	292	295	rBV	7103817	8239940	87.98%	9.740%
3	6.453	379	382	385	rVB	6087508	9366159	100.00%	11.071%
4	6.590	391	394	396	rBV	6654387	9328047	99.59%	11.026%
5	6.807	411	413	416	rBV	1773414	1899054	20.28%	2.245%
6	6.967	424	427	430	rBV	6493893	6271566	66.96%	7.413%
7	7.379	460	463	465	rBV	5603097	6007726	64.14%	7.101%
8	7.482	468	472	480	rVB	151831	216844	2.32%	0.256%
9	8.099	523	526	528	rBV	2723818	2683505	28.65%	3.172%
10	9.173	617	620	623	rBV	7444974	7869902	84.02%	9.303%
11	9.425	639	642	648	rBV	253577	393721	4.20%	0.465%
12	9.573	652	655	657	rBV	3336178	3036613	32.42%	3.589%
13	9.848	676	679	681	rBV	3145736	2761771	29.49%	3.265%
14	10.110	700	702	704	rBV	127797	111174	1.19%	0.131%
15	10.293	714	718	719	rBV2	131236	222856	2.38%	0.263%
16	10.511	734	737	738	rBV	81125	117051	1.25%	0.138%
17	10.636	745	748	751	rBV	5119297	5233332	55.87%	6.186%
18	10.762	757	759	765	rVB	262228	327105	3.49%	0.387%
19	11.173	793	795	796	rBV	361500	373866	3.99%	0.442%
20	11.208	796	798	799	rBV	174922	142607	1.52%	0.169%
21	11.333	806	809	811	rBV	2097843	2632800	28.11%	3.112%
22	11.871	854	856	857	rBV	280713	357321	3.82%	0.422%
23	12.922	945	948	950	rBV	5806767	7697019	82.18%	9.098%
24	13.814	1024	1026	1028	rBV	635326	659793	7.04%	0.780%
25	13.962	1036	1039	1041	rBV	1843252	2313094	24.70%	2.734%
26	14.454	1079	1082	1085	rVB2	51181	99877	1.07%	0.118%
27	14.808	1111	1113	1117	rBV2	53611	107048	1.14%	0.127%
28	15.368	1159	1162	1165	rBV	1229458	1740978	18.59%	2.058%
29	15.608	1180	1183	1190	rVB3	39162	107350	1.15%	0.127%
30	15.825	1199	1202	1205	rBV	64461	114199	1.22%	0.135%
31	16.305	1241	1244	1250	rVB2	46260	93990	1.00%	0.111%
32	16.808	1284	1288	1290	rBV	80707	151933	1.62%	0.180%
33	17.300	1328	1331	1338	rVB8	39767	98405	1.05%	0.116%
34	19.220	1495	1499	1510	rVB6	65176	272937	2.91%	0.323%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121316\
Data File : BF091549.D
Acq On : 13 Dec 2016 13:04
Operator : UM/SJ
Sample : H5940-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS06-0-2IN

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-BF120916.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 84599531

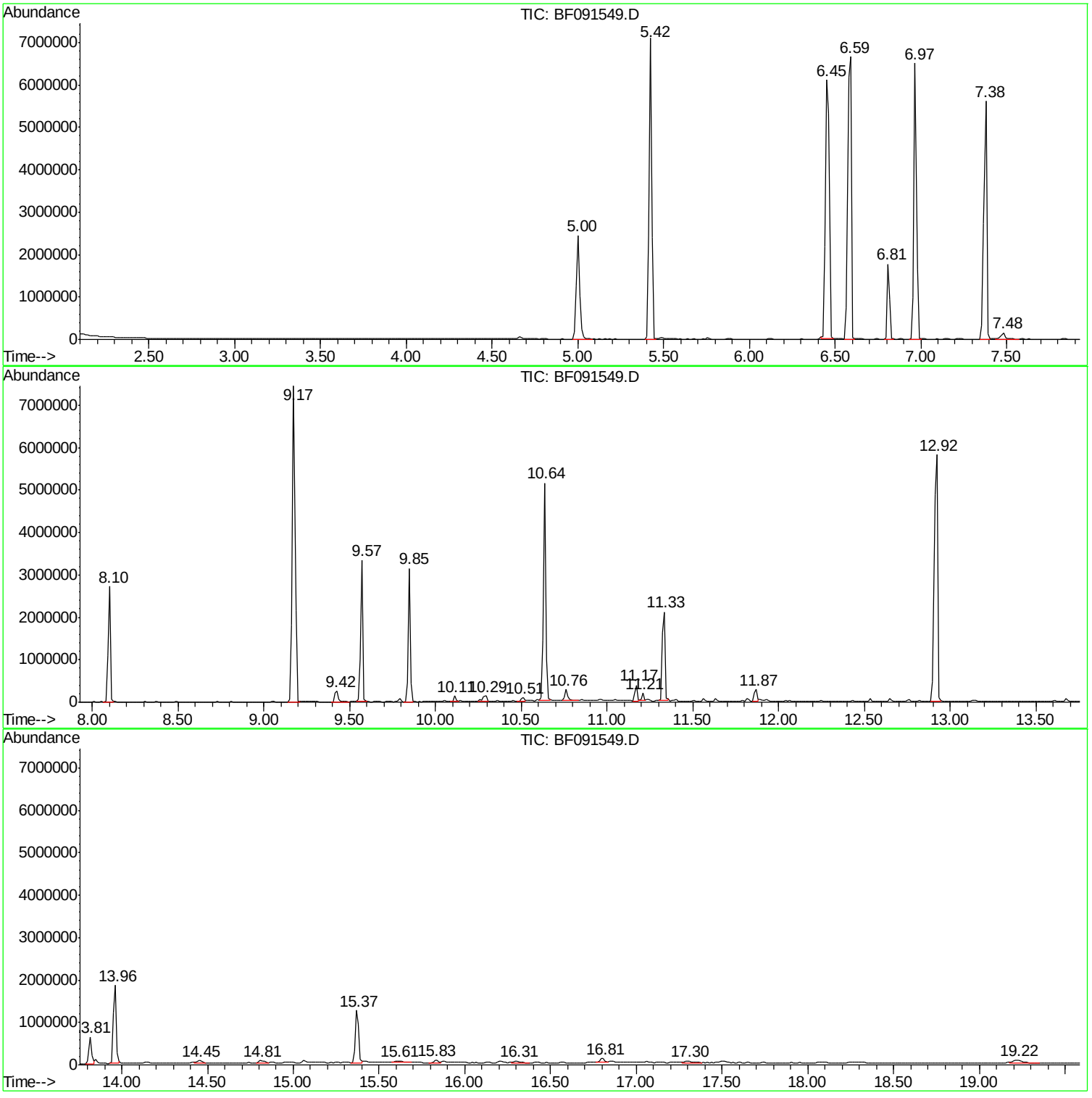
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121316\
Data File : BF091549.D
Acq On : 13 Dec 2016 13:04
Operator : UM/SJ
Sample : H5940-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS06-0-2IN

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121316\
Data File : BF091549.D
Acq On : 13 Dec 2016 13:04
Operator : UM/SJ
Sample : H5940-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS06-0-2IN

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

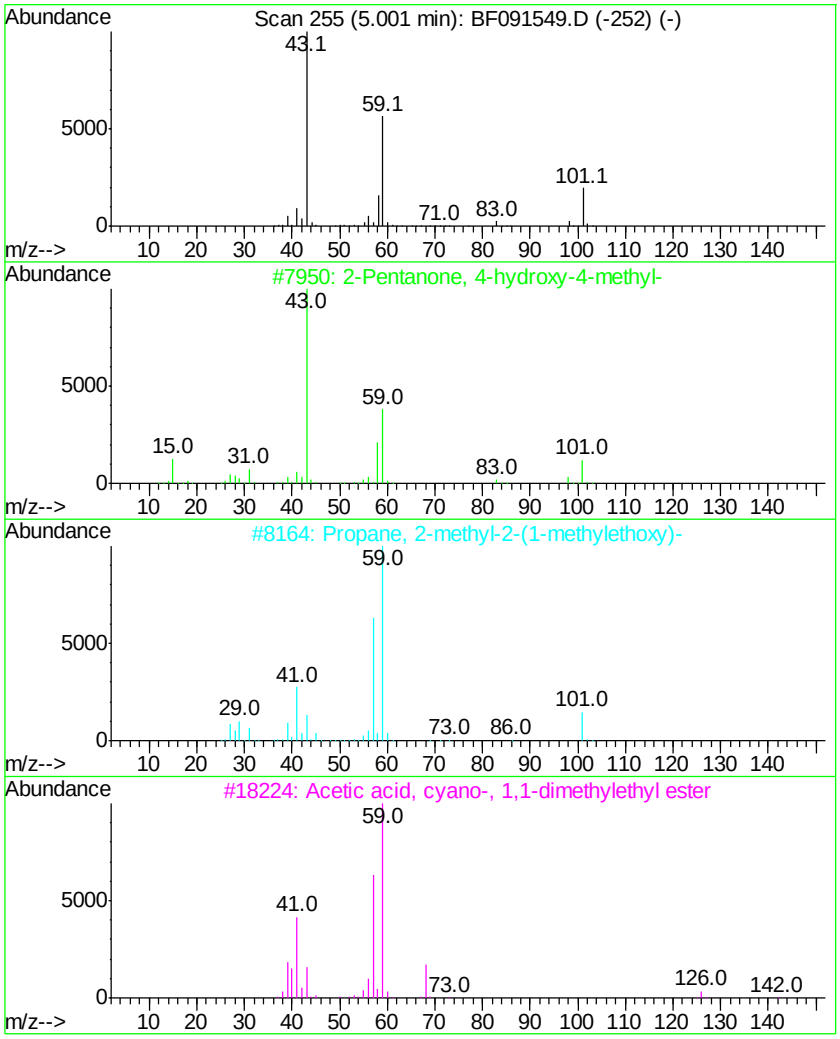
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

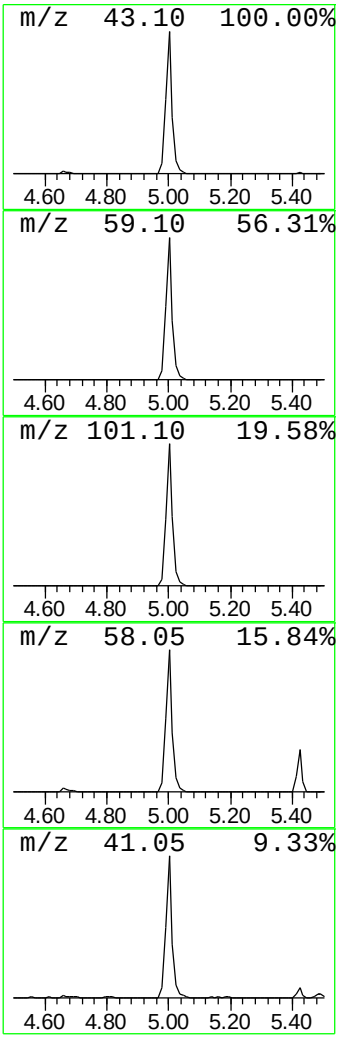
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	37.39 ng	3549950	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	53
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121316\
Data File : BF091549.D
Acq On : 13 Dec 2016 13:04
Operator : UM/SJ
Sample : H5940-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS06-0-2IN

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

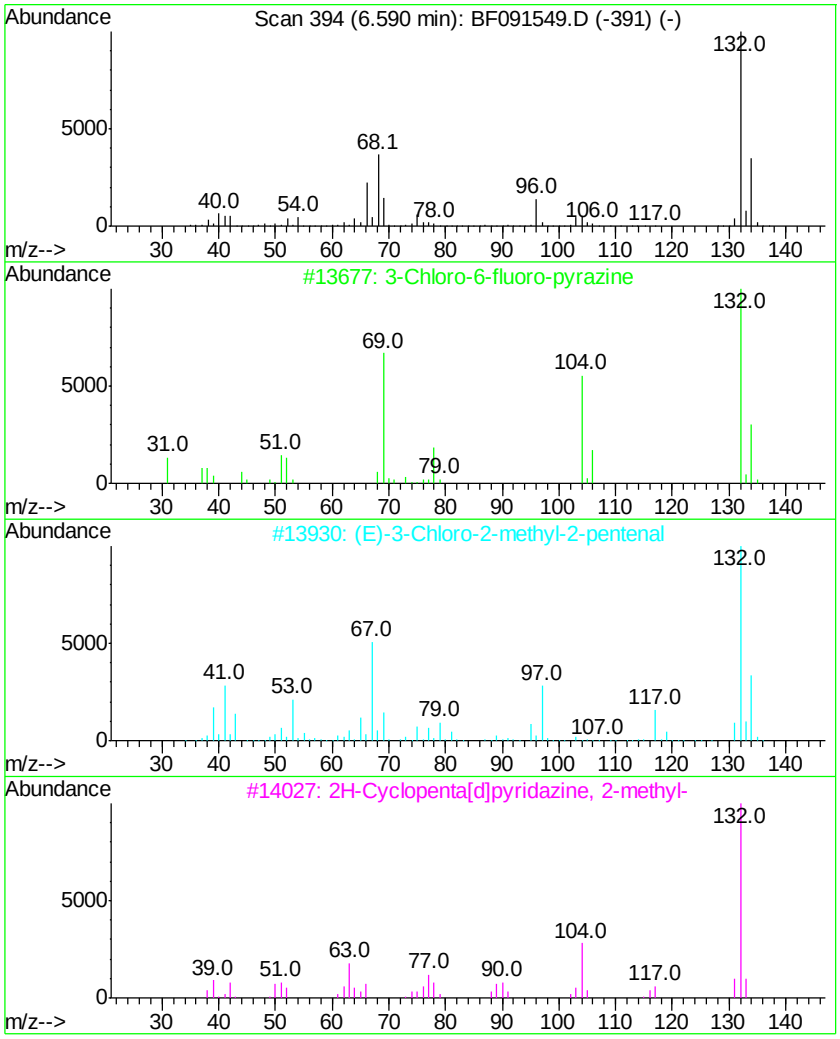
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

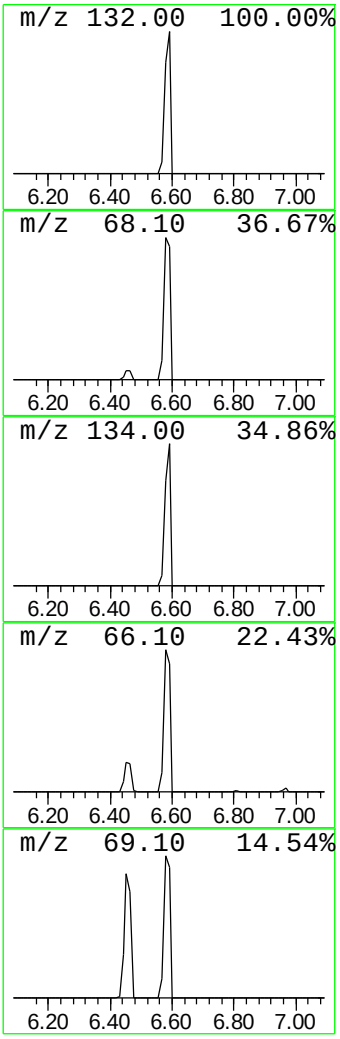
****

Peak Number 2 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	98.24 ng	9328050	1,4-Dichlorobenzene-d4	6.81

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	17
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121316\
Data File : BF091549.D
Acq On : 13 Dec 2016 13:04
Operator : UM/SJ
Sample : H5940-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS06-0-2IN

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

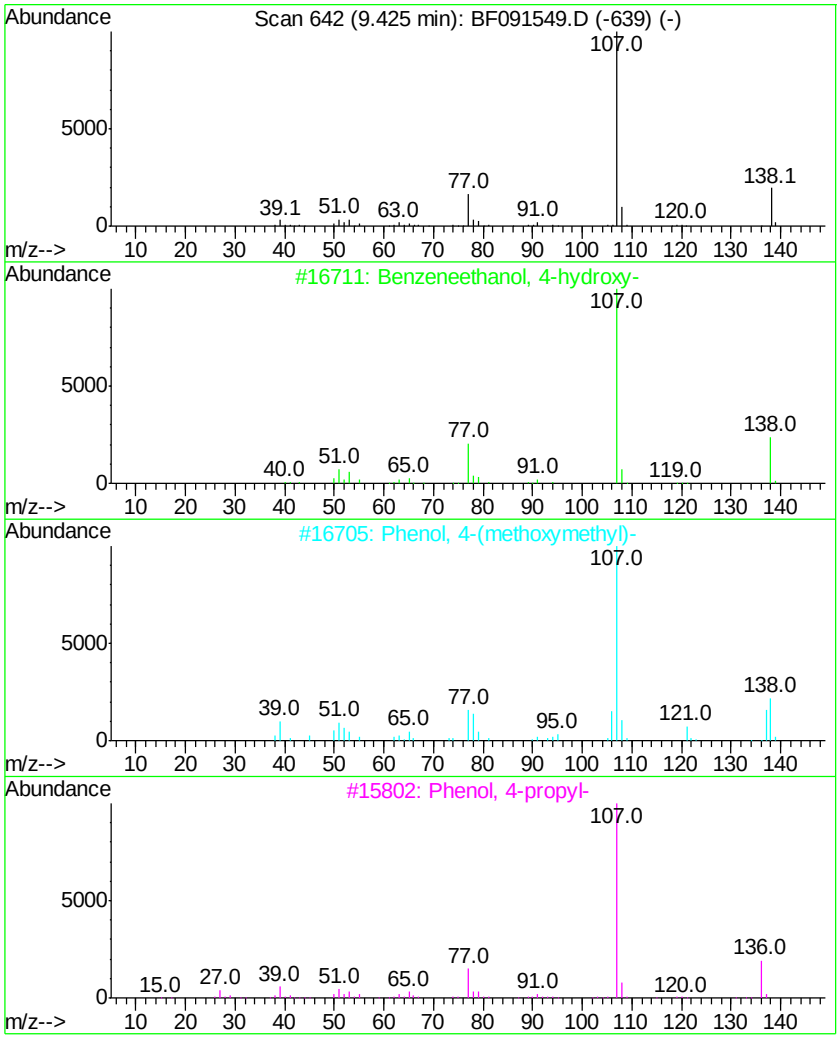
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

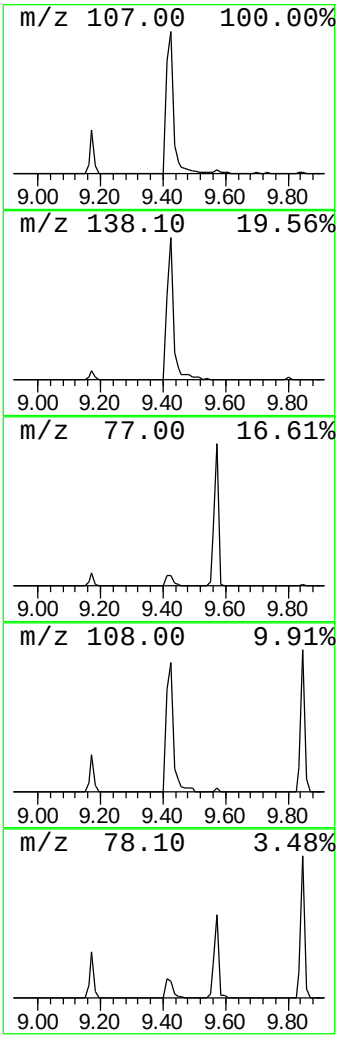
****

Peak Number 4 Benzeneethanol, 4-hydroxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.42	2.85 ng	393721	Acenaphthene-d10	9.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneethanol, 4-hydroxy-	138	C8H10O2	000501-94-0	90
2	Phenol, 4-(methoxymethyl)-	138	C8H10O2	005355-17-9	78
3	Phenol, 4-propyl-	136	C9H12O	000645-56-7	59
4	Pyridine, 2,5-dimethyl-	107	C7H9N	000589-93-5	53
5	Phenol, 2-propyl-	136	C9H12O	000644-35-9	45





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121316\
Data File : BF091549.D
Acq On : 13 Dec 2016 13:04
Operator : UM/SJ
Sample : H5940-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS06-0-2IN

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

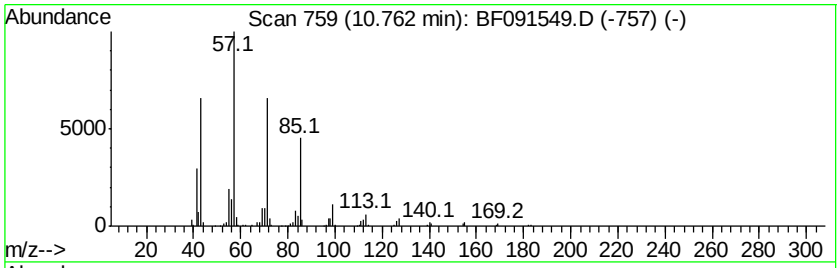
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

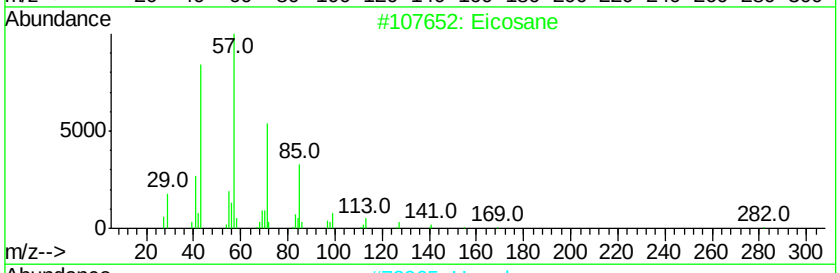
****

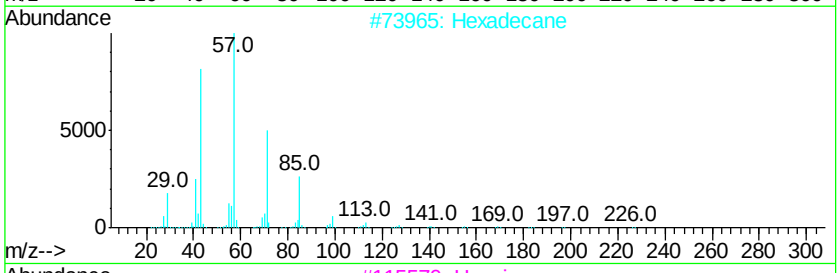
Peak Number 5 Eicosane Concentration Rank 9

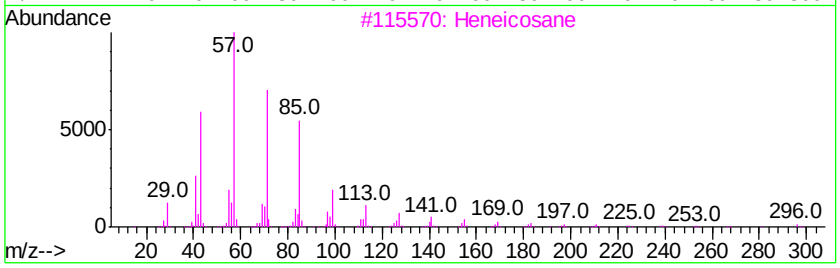
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.76	2.48 ng	327105	Phenanthrene-d10	11.33

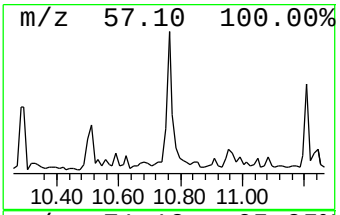
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86

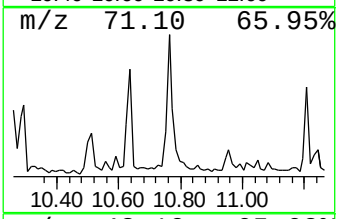


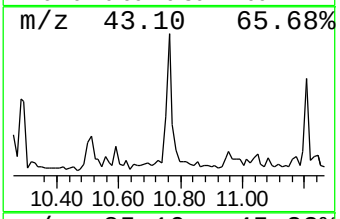


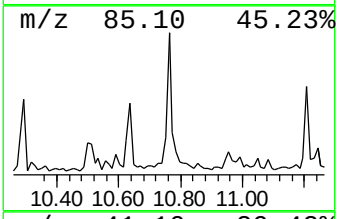


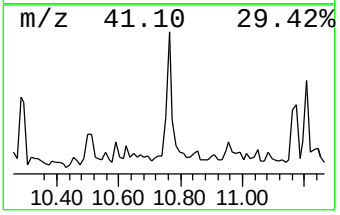












Data Path : Z:\HPCHEM1\BNA F\DATA\BF121316\
Data File : BF091549.D
Acq On : 13 Dec 2016 13:04
Operator : UM/SJ
Sample : H5940-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS06-0-2IN

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

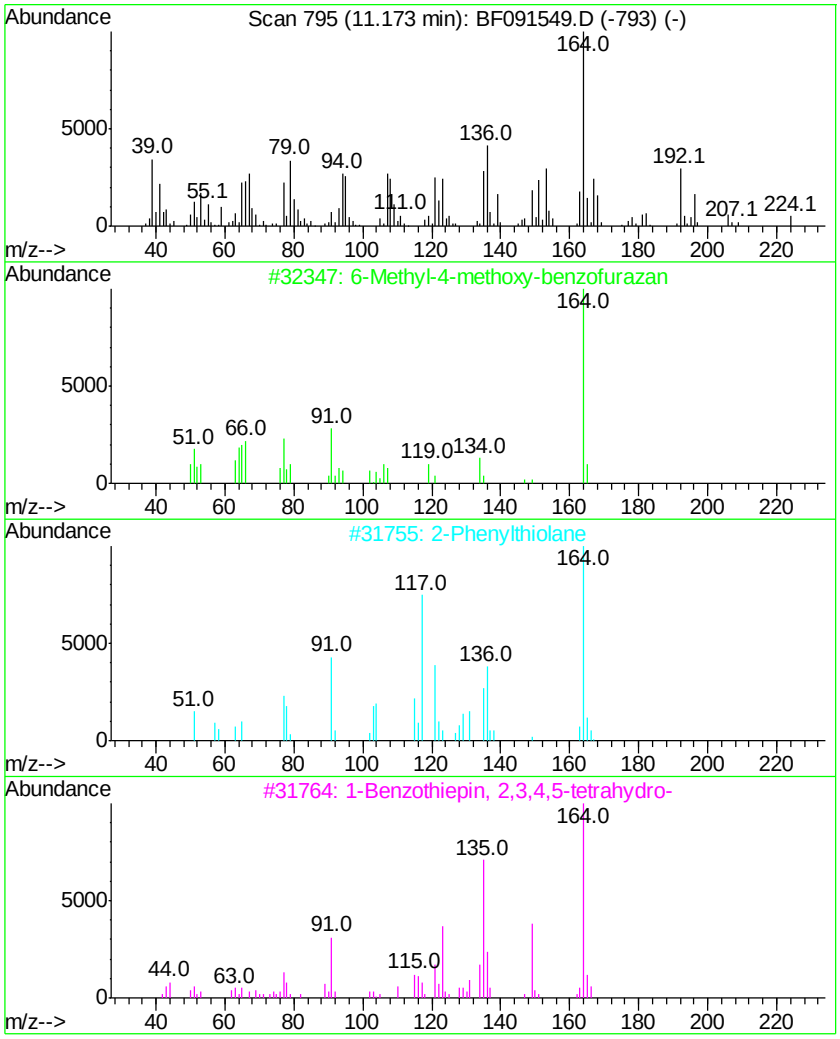
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

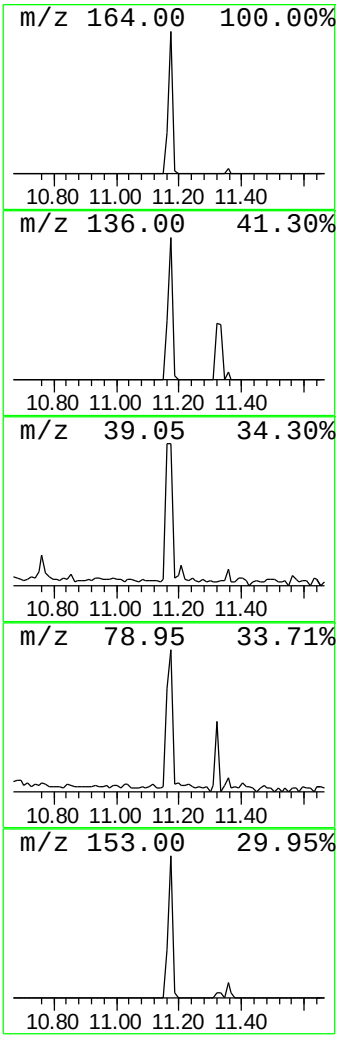
****

Peak Number 6 unknown11.17 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.17	2.84 ng	373866	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Methyl-4-methoxy-benzofurazan	164	C8H8N2O2	063006-67-7	38
2	2-Phenylthiolane	164	C10H12S	002060-65-3	30
3	1-Benzothiepin, 2,3,4,5-tetrahydro-	164	C10H12S	004370-78-9	27
4	2(3H)-Benzothiazolimine, 3-methyl-	164	C8H8N2S	014779-16-9	22
5	2,5-Cyclohexadiene-1,4-dione, 2-...	164	C10H12O2	000490-91-5	22





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121316\
Data File : BF091549.D
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Sample : H5940-06
Misc :
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Instrument : BNA_F
ClientSampleId : SS06-0-2IN

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

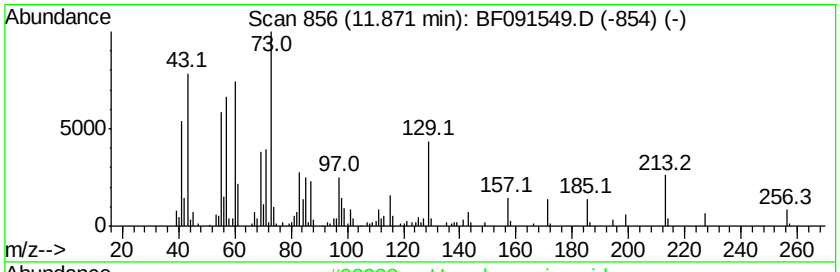
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

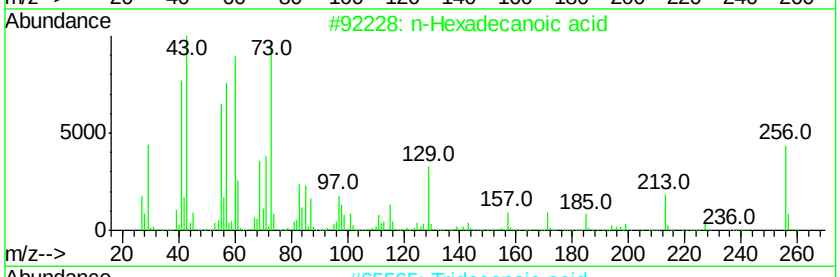
****

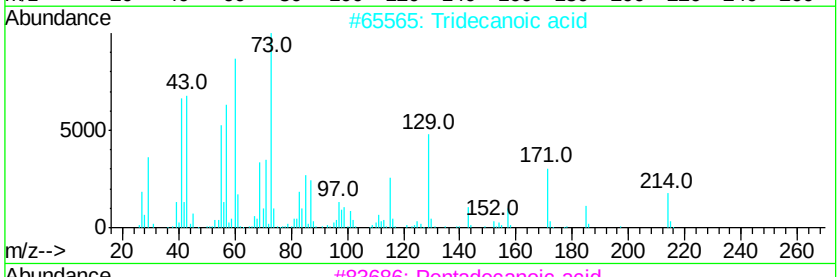
Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

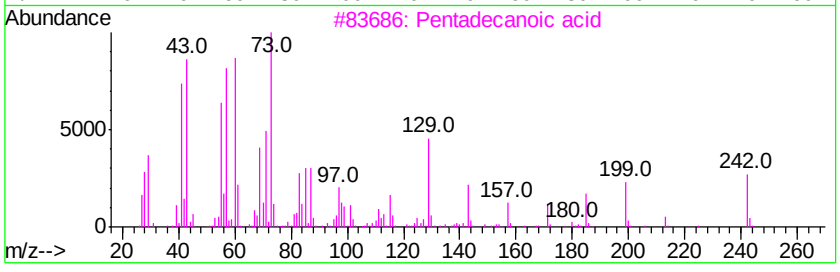
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	2.71 ng	357321	Phenanthrene-d10	11.33

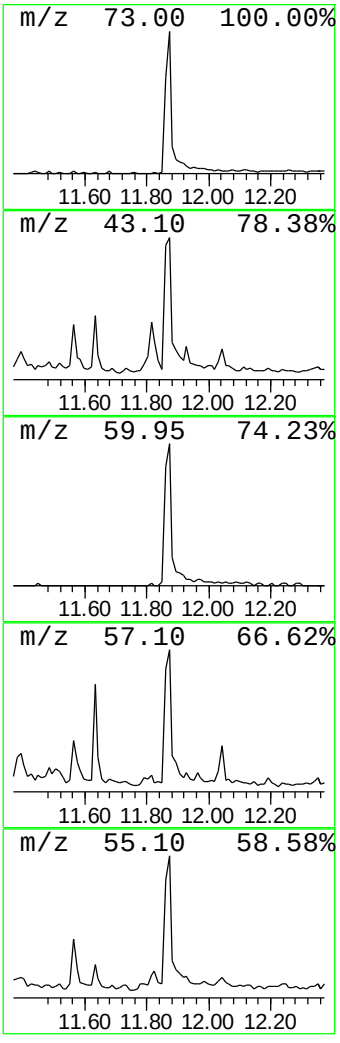
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	n-Decanoic acid	172	C10H20O2	000334-48-5	68
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	38











Data Path : Z:\HPCHEM1\BNA F\DATA\BF121316\
Data File : BF091549.D
Acq On : 13 Dec 2016 13:04
Operator : UM/SJ
Sample : H5940-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS06-0-2IN

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

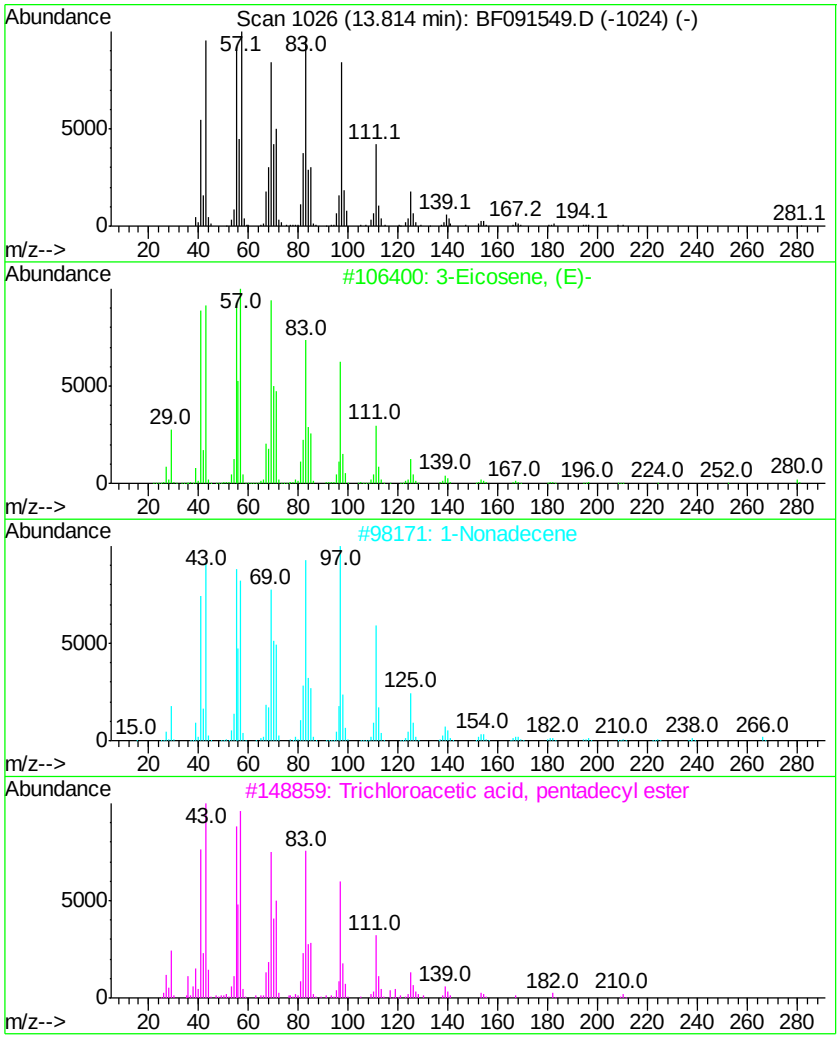
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

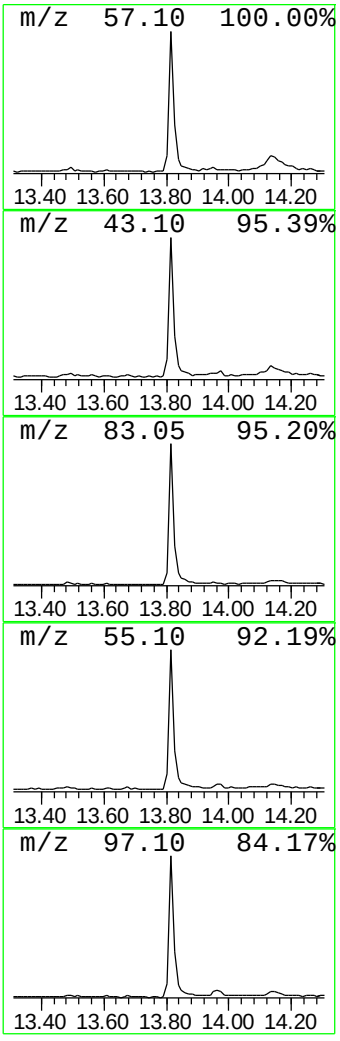
****

Peak Number 8 3-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	5.70 ng	659793	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
4	Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	90
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121316\
Data File : BF091549.D
Acq On : 13 Dec 2016 13:04
Operator : UM/SJ
Sample : H5940-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS06-0-2IN

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

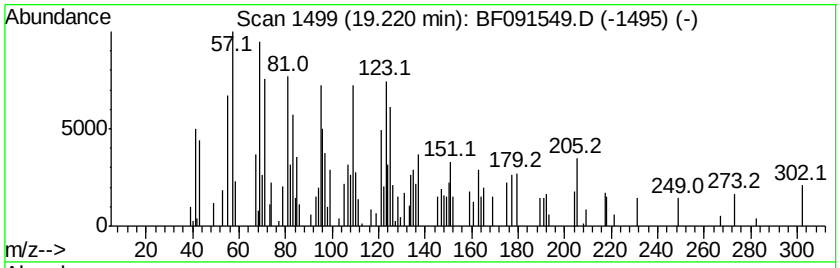
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

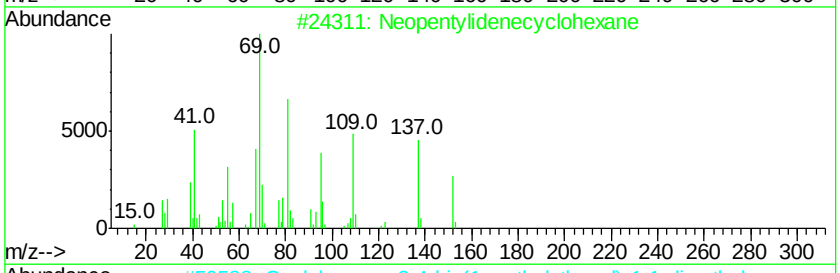
****

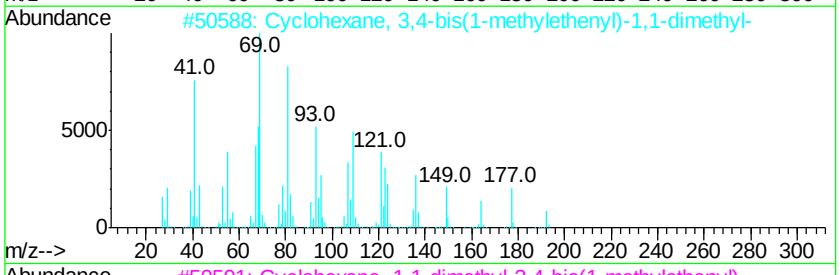
Peak Number 9 Neopentylidenecyclohexane Concentration Rank 5

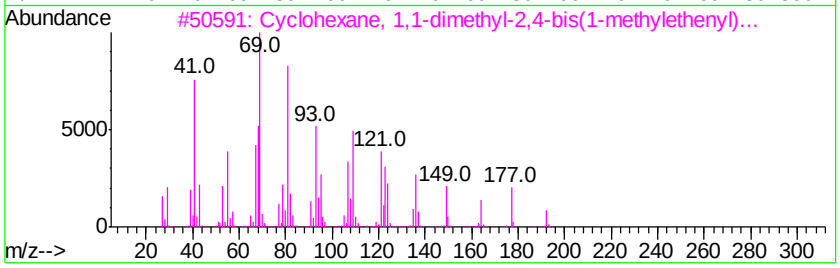
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.22	3.14 ng	272937	Perylene-d12	15.37

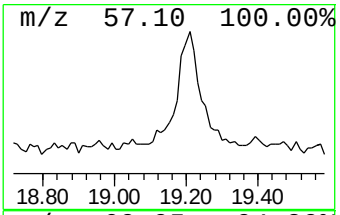
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Neopentylidenecyclohexane	152	C11H20	039546-80-0	50
2	Cyclohexane, 3,4-bis(1-methyleth...	192	C14H24	061142-74-3	38
3	Cyclohexane, 1,1-dimethyl-2,4-bi...	192	C14H24	062337-98-8	38
4	3-Cyclopentylpropionic acid, 3-c...	216	C11H17ClO2	1000292-47-2	27
5	Sesquirosefuran	218	C15H22O	039007-93-7	27

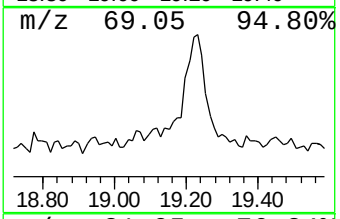


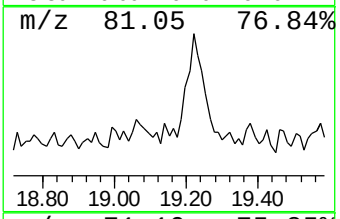


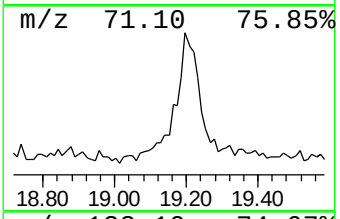


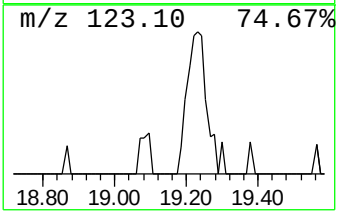












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121316\
Data File : BF091549.D
Acq On : 13 Dec 2016 13:04
Operator : UM/SJ
Sample : H5940-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS06-0-2IN

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.00	37.4	ng	3549950	1	6.81	1899050	20.0
unknown6.59	6.59	98.2	ng	9328050	1	6.81	1899050	20.0
Benzeneethanol, 4...	9.42	2.9	ng	393721	3	9.85	2761770	20.0
Eicosane	10.76	2.5	ng	327105	4	11.33	2632800	20.0
unknown11.17	11.17	2.8	ng	373866	4	11.33	2632800	20.0
n-Hexadecanoic acid	11.87	2.7	ng	357321	4	11.33	2632800	20.0
3-Eicosene, (E)-	13.81	5.7	ng	659793	5	13.96	2313090	20.0
Neopentylidenecyc...	19.22	3.1	ng	272937	6	15.37	1740980	20.0