LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094257.D
Acq On : 7 Apr 2017 6:55
Operator : SJ/MA
Sample : I2542-14
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-1

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-BF032217.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	3.999	354	359	369	rBV	748466	1054615	21.21%	2.626%
2	4.399	421	427	430	rBV	4119759	4465924	89.80%	11.121%
3	4.781	488	492	496	rVB	65980	60510	1.22%	0.151%
4	5.469	602	609	614	rBV2	3596224	4973060	100.00%	12.384%
5	5.604	626	632	635	rBV	4208848	4710616	94.72%	11.731%
6	5.851	670	674	678	rBV	1081624	971886	19.54%	2.420%
7	6.034	700	705	708	rBV	3553521	3548202	71.35%	8.836%
8	6.504	778	785	788	rBV	2478799	3066030	61.65%	7.635%
9	7.357	924	930	933	rBV	1310007	1282809	25.80%	3.195%
10	8.681	1149	1155	1159	rBV	4103576	4606784	92.63%	11.472%
11	9.175	1234	1239	1245	rBV	401533	366284	7.37%	0.912%
12	9.492	1284	1293	1302	rBV2	1256672	1357496	27.30%	3.381%
13	10.086	1391	1394	1398	rVB	58690	57814	1.16%	0.144%
14	10.469	1453	1459	1463	rBV	2140716	2550809	51.29%	6.352%
15	10.675	1490	1494	1504	rBV	89494	118820	2.39%	0.296%
16	11.227	1584	1588	1592	rBV	71643	67518	1.36%	0.168%
17	11.316	1599	1603	1607	rBV	1146206	1162395	23.37%	2.895%
18	12.810	1853	1857	1862	rVB	54370	52740	1.06%	0.131%
19	13.086	1899	1904	1909	rBV	43745	50614	1.02%	0.126%
20	13.298	1934	1940	1944	rBV	2634923	3124753	62.83%	7.782%
21	14.463	2134	2138	2148	rBV2	243433	396040	7.96%	0.986%
22	14.568	2151	2156	2160	rBV	885469	872017	17.53%	2.172%
23	14.868	2203	2207	2212	rBV	67508	73282	1.47%	0.182%
24	15.251	2268	2272	2279	rBV2	94781	142304	2.86%	0.354%
25	15.610	2330	2333	2338	rBV	58234	77408	1.56%	0.193%
26	15.962	2390	2393	2400	rVB	76204	83658	1.68%	0.208%
27	16.198	2428	2433	2442	rBV	665806	790385	15.89%	1.968%
28	16.721	2518	2522	2526	rBV2	47938	71017	1.43%	0.177%

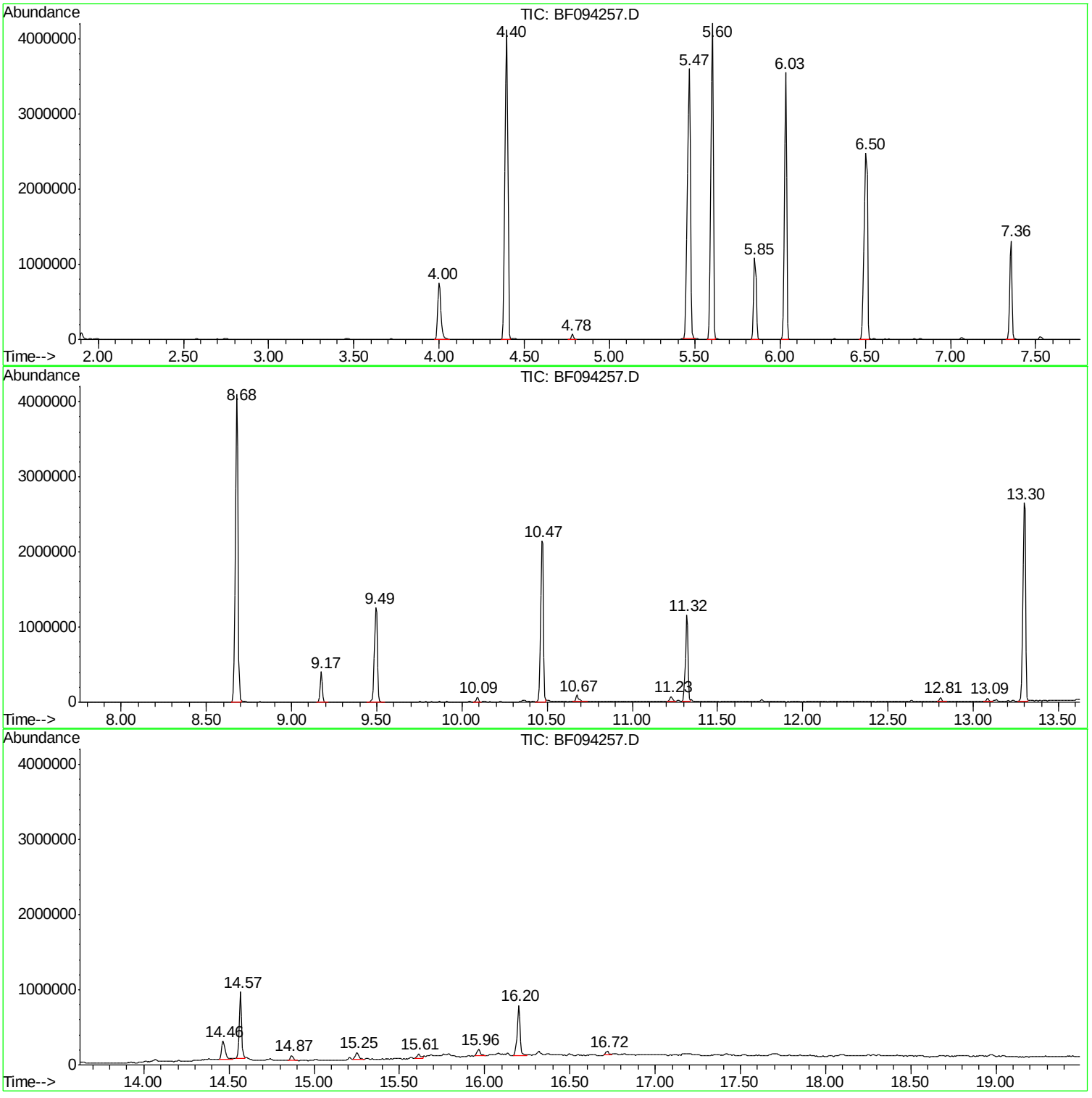
Sum of corrected areas: 40155790

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094257.D
Acq On : 7 Apr 2017 6:55
Operator : SJ/MA
Sample : I2542-14
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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\BF040617\
Data File : BF094257.D
Acq On : 7 Apr 2017 6:55
Operator : SJ/MA
Sample : I2542-14
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

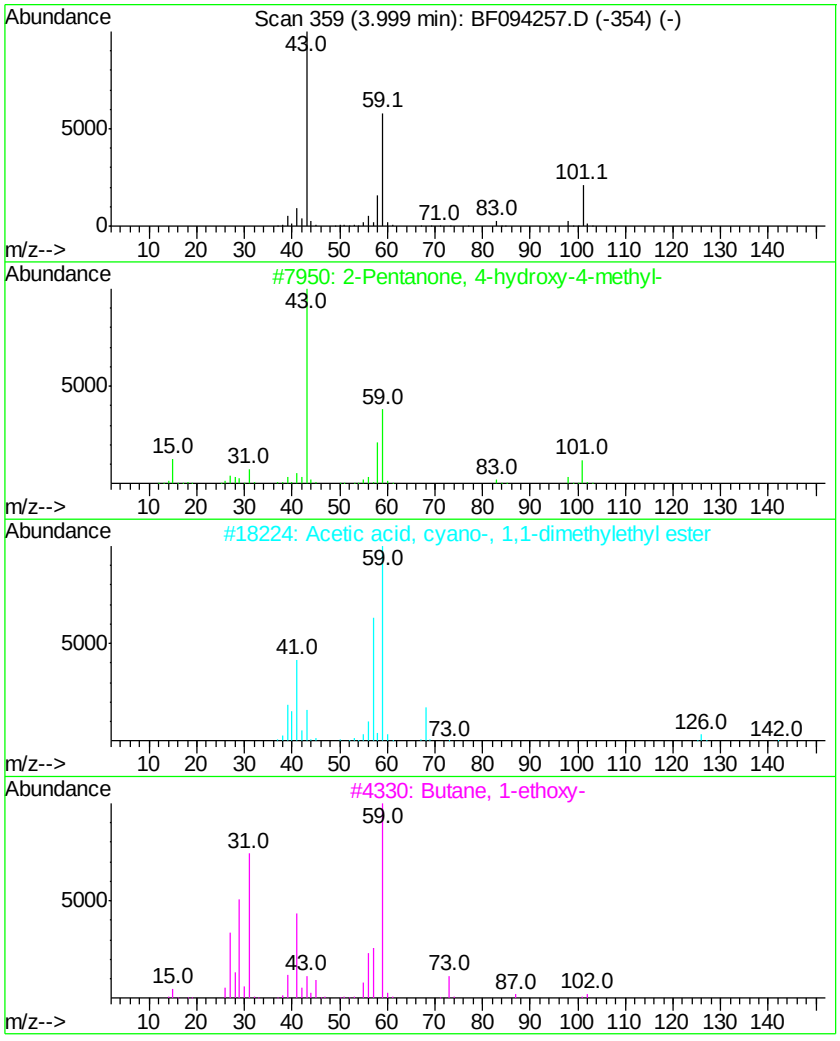
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

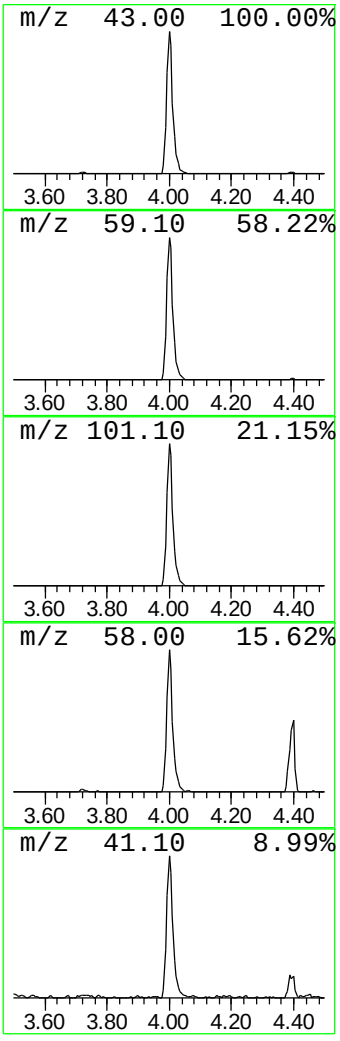
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.00	21.70 ng	1054620	1,4-Dichlorobenzene-d4	5.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094257.D
Acq On : 7 Apr 2017 6:55
Operator : SJ/MA
Sample : I2542-14
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

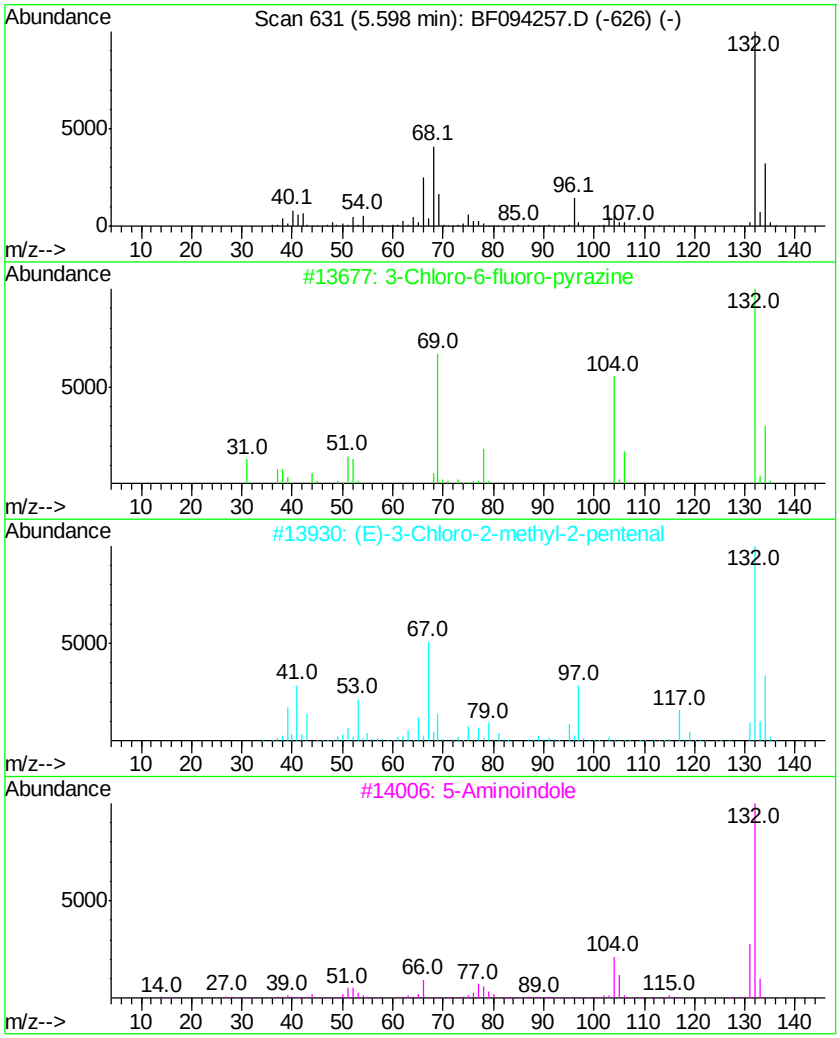
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

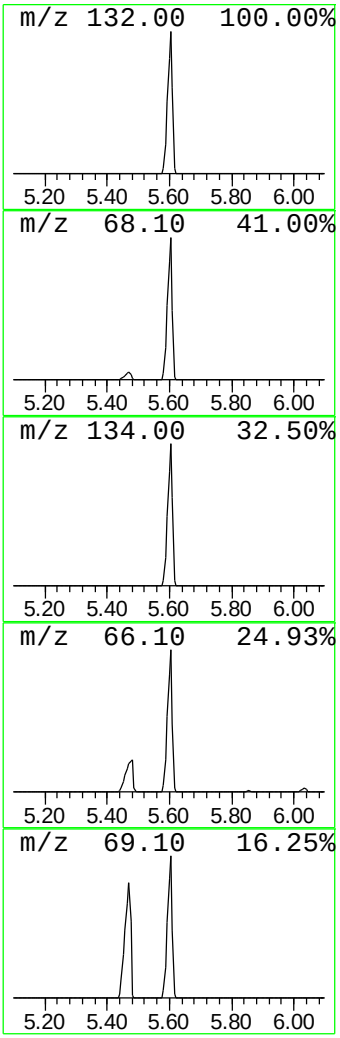
****

Peak Number 2 unknown5.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.60	96.94 ng	4710620	1,4-Dichlorobenzene-d4	5.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094257.D
Acq On : 7 Apr 2017 6:55
Operator : SJ/MA
Sample : I2542-14
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

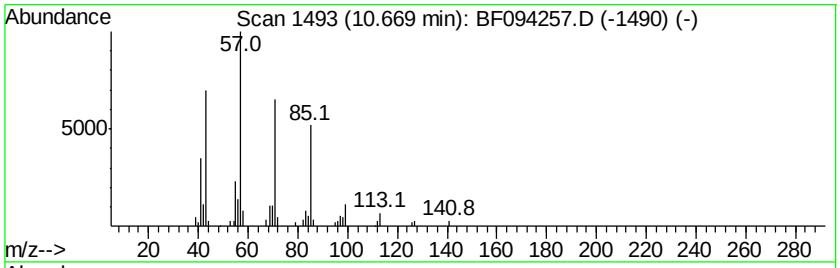
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

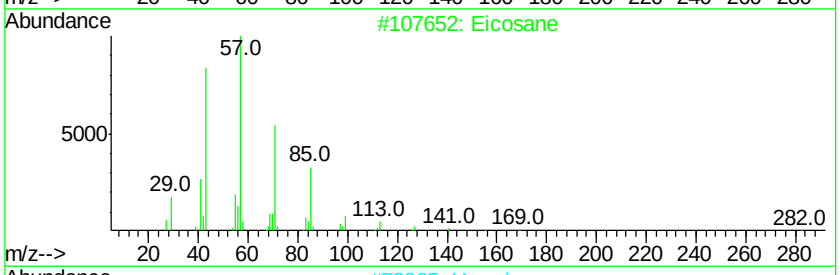
****

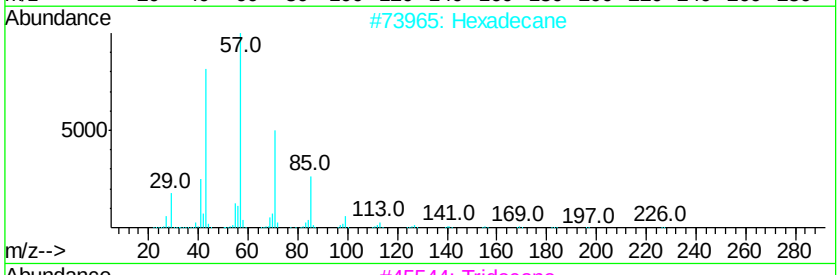
Peak Number 4 Eicosane Concentration Rank 7

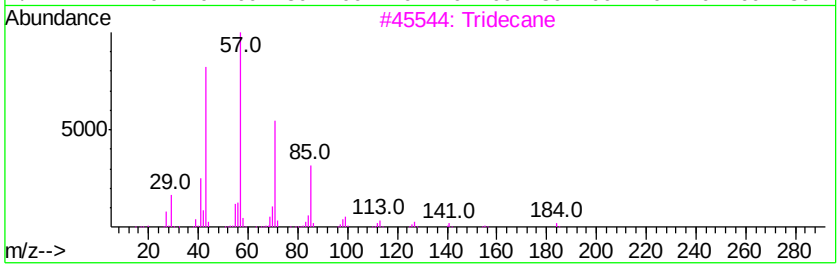
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	2.04 ng	118820	Phenanthrene-d10	11.32

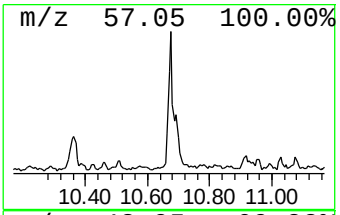
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Tridecane	184	C13H28	000629-50-5	90
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83
5	Octadecane	254	C18H38	000593-45-3	78

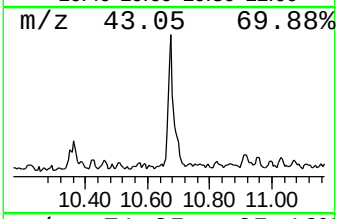


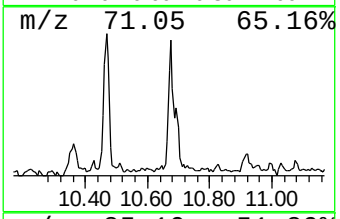


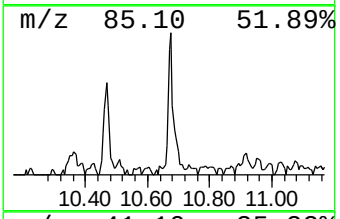


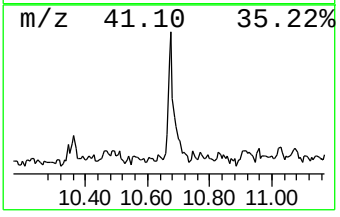












Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094257.D
Acq On : 7 Apr 2017 6:55
Operator : SJ/MA
Sample : I2542-14
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

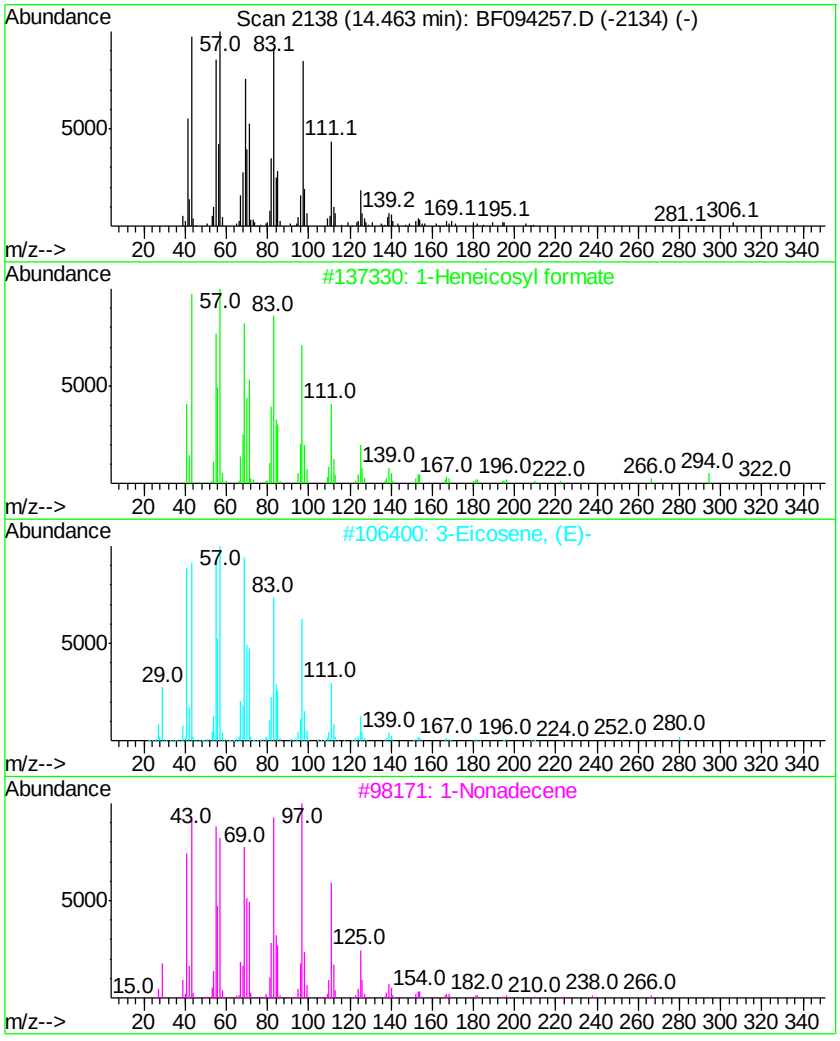
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

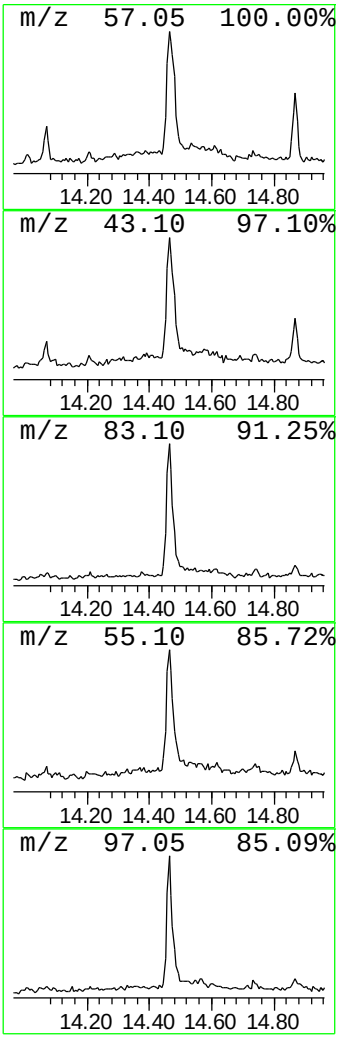
****

Peak Number 5 1-Heneicosyl formate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.46	9.08 ng	396040	Chrysene-d12	14.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094257.D
Acq On : 7 Apr 2017 6:55
Operator : SJ/MA
Sample : I2542-14
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

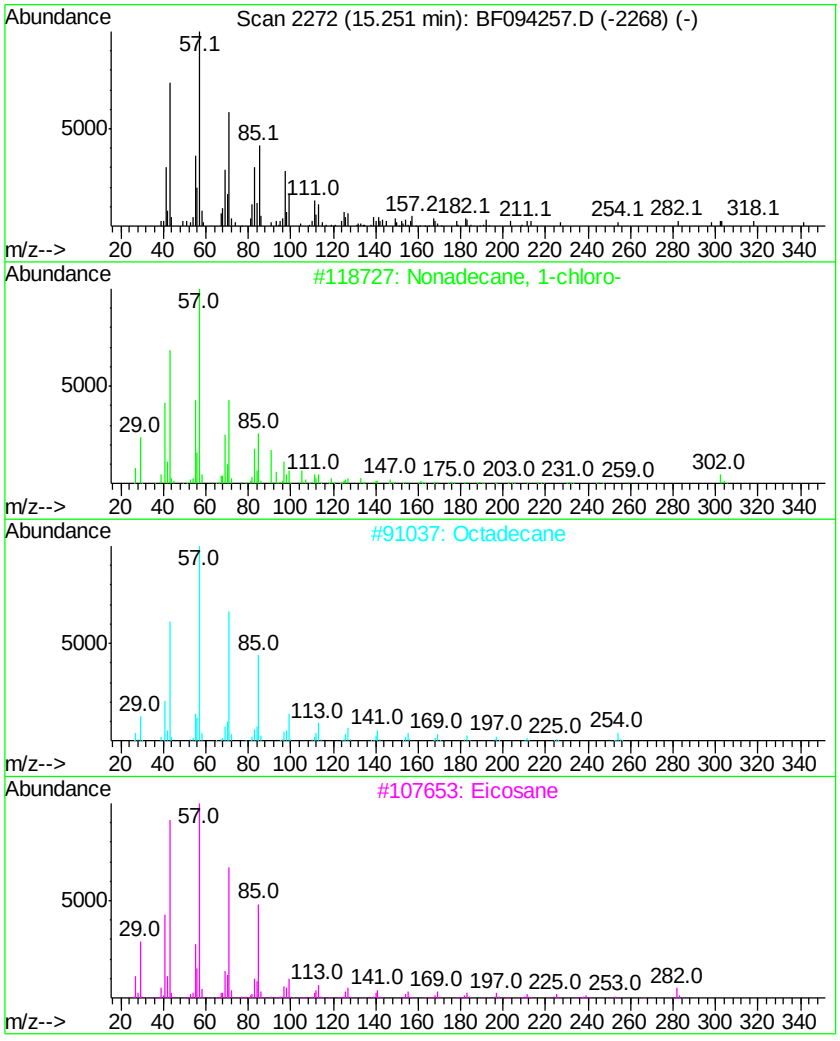
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

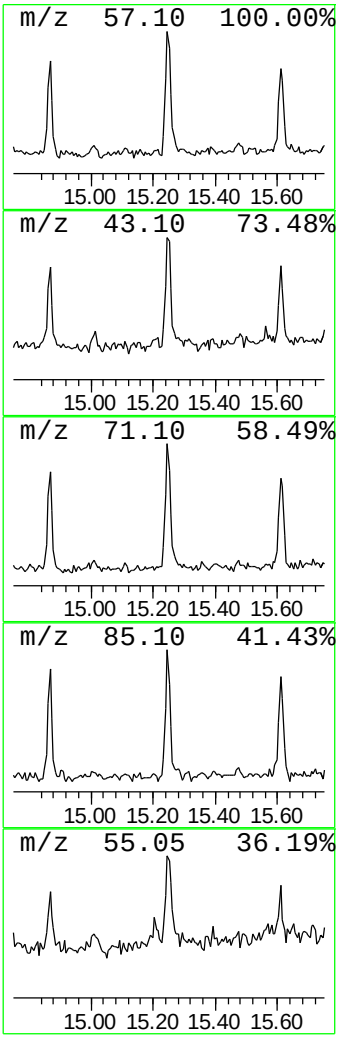
****

Peak Number 6 Nonadecane, 1-chloro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.25	3.26 ng	142304	Chrysene-d12	14.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	95
2	Octadecane	254	C18H38	000593-45-3	92
3	Eicosane	282	C20H42	000112-95-8	89
4	Tetracosane, 1-bromo-	416	C24H49Br	006946-24-3	83
5	Tetradecane	198	C14H30	000629-59-4	68





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094257.D
Acq On : 7 Apr 2017 6:55
Operator : SJ/MA
Sample : I2542-14
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

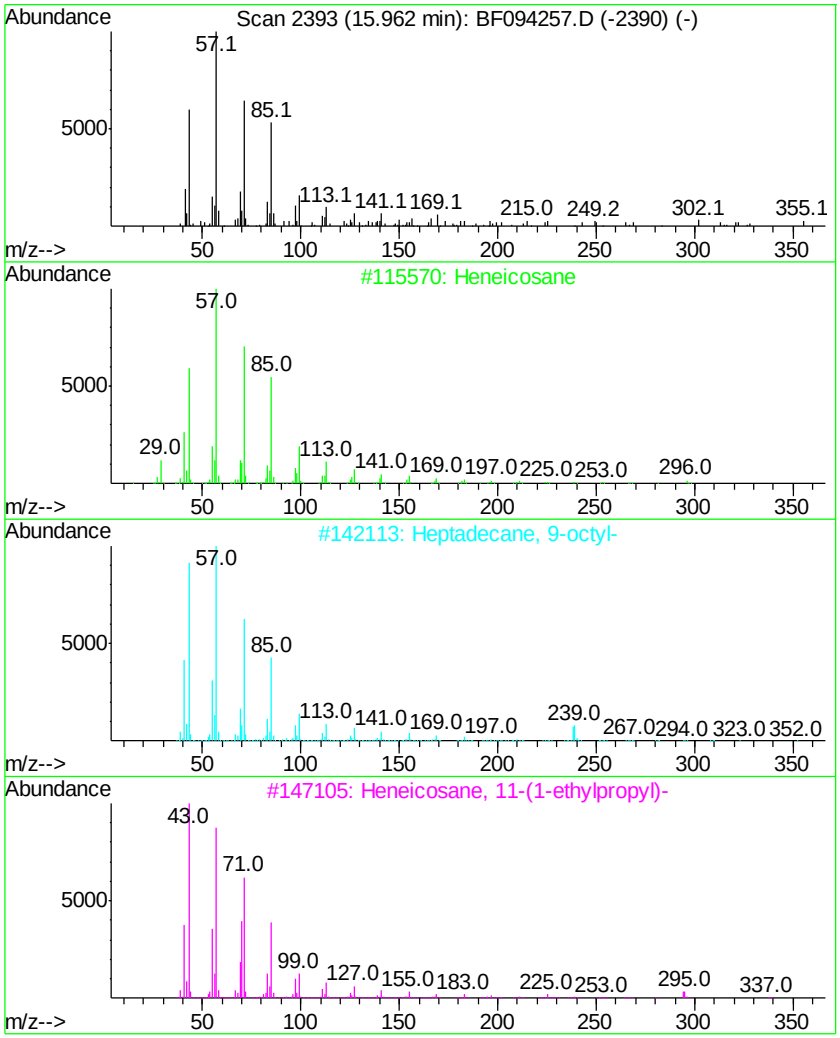
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

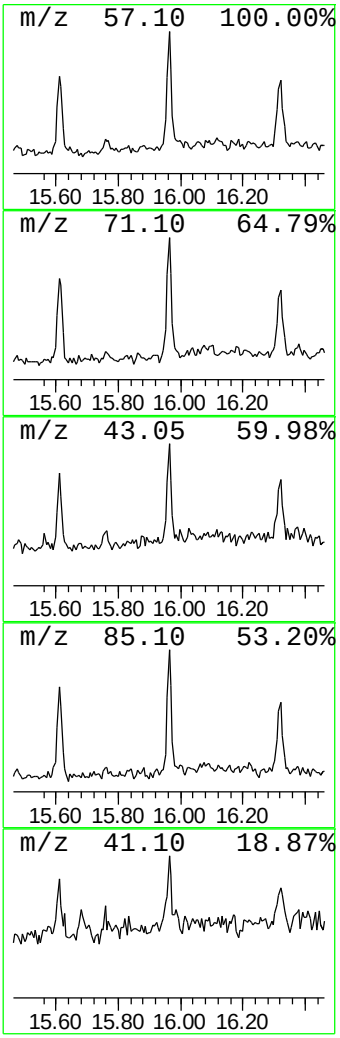
****

Peak Number 7 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	2.12 ng	83658	Perylene-d12	16.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	87
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87
4	Nonacosane	408	C29H60	000630-03-5	86
5	Triacontane	422	C30H62	000638-68-6	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040617\
Data File : BF094257.D
Acq On : 7 Apr 2017 6:55
Operator : SJ/MA
Sample : I2542-14
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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...	4.00	21.7	ng	1054620	1	5.85	971886	20.0
unknown5.60	5.60	96.9	ng	4710620	1	5.85	971886	20.0
Eicosane	10.67	2.0	ng	118820	4	11.32	1162400	20.0
1-Heneicosyl formate	14.46	9.1	ng	396040	5	14.57	872017	20.0
Nonadecane, 1-chl...	15.25	3.3	ng	142304	5	14.57	872017	20.0
Heneicosane	15.96	2.1	ng	83658	6	16.20	790385	20.0