LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051117\
Data File : BF095096.D
Acq On : 11 May 2017 23:53
Operator : SJ/MA
Sample : I3087-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01_001

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-BF050217.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	5.007	517	522	541	rBV	338332	708458	25.76%	3.206%
2	5.648	627	631	659	rBV	1118180	1974554	71.79%	8.935%
3	6.225	725	729	738	rBV	20231	34301	1.25%	0.155%
4	7.248	899	903	918	rBV	1287321	1944001	70.68%	8.797%
5	7.366	918	923	942	rVB	1597580	2314531	84.15%	10.473%
6	7.701	976	980	991	rBV	391855	469019	17.05%	2.122%
7	7.942	1016	1021	1036	rBV	1377999	1708751	62.13%	7.732%
8	8.601	1129	1133	1158	rBV	897007	1305202	47.46%	5.906%
9	9.725	1319	1324	1346	rBV	458846	675560	24.56%	3.057%
10	11.495	1620	1625	1639	rBV	2166655	2750333	100.00%	12.445%
11	12.189	1739	1743	1755	rBV	267102	352457	12.82%	1.595%
12	12.554	1800	1805	1816	rBV2	545888	791233	28.77%	3.580%
13	13.395	1943	1948	1953	rVB	40233	46873	1.70%	0.212%
14	13.848	2020	2025	2039	rBV	950072	1484640	53.98%	6.718%
15	14.165	2075	2079	2082	rBV	44397	53134	1.93%	0.240%
16	14.895	2199	2203	2208	rBV	27542	33821	1.23%	0.153%
17	14.954	2208	2213	2231	rVB	544063	808329	29.39%	3.658%
18	15.924	2373	2378	2387	rBV2	139110	179900	6.54%	0.814%
19	17.012	2559	2563	2569	rBV2	29574	45221	1.64%	0.205%
20	17.283	2603	2609	2621	rBV	2266292	2625164	95.45%	11.879%
21	18.547	2817	2824	2833	rBV5	34357	121340	4.41%	0.549%
22	18.624	2833	2837	2845	rVV	461738	605957	22.03%	2.742%
23	19.753	3025	3029	3033	rBV	45128	53551	1.95%	0.242%
24	20.036	3073	3077	3085	rVB3	37172	48742	1.77%	0.221%
25	20.294	3117	3121	3132	rVB	358971	510419	18.56%	2.310%
26	20.747	3189	3198	3202	rBV6	20433	42062	1.53%	0.190%
27	22.065	3416	3422	3429	rBV9	34607	75435	2.74%	0.341%
28	22.177	3438	3441	3447	rVB7	21101	40451	1.47%	0.183%
29	22.306	3455	3463	3468	rBV10	14490	46684	1.70%	0.211%
30	22.459	3483	3489	3492	rBV8	19625	39358	1.43%	0.178%
31	22.871	3553	3559	3565	rVB6	27981	63071	2.29%	0.285%
32	23.582	3669	3680	3681	rBV7	23291	54555	1.98%	0.247%
33	23.694	3693	3699	3706	rVB7	38309	92123	3.35%	0.417%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051117\
Data File : BF095096.D
Acq On : 11 May 2017 23:53
Operator : SJ/MA
Sample : I3087-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01_001

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-BF050217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 22099230

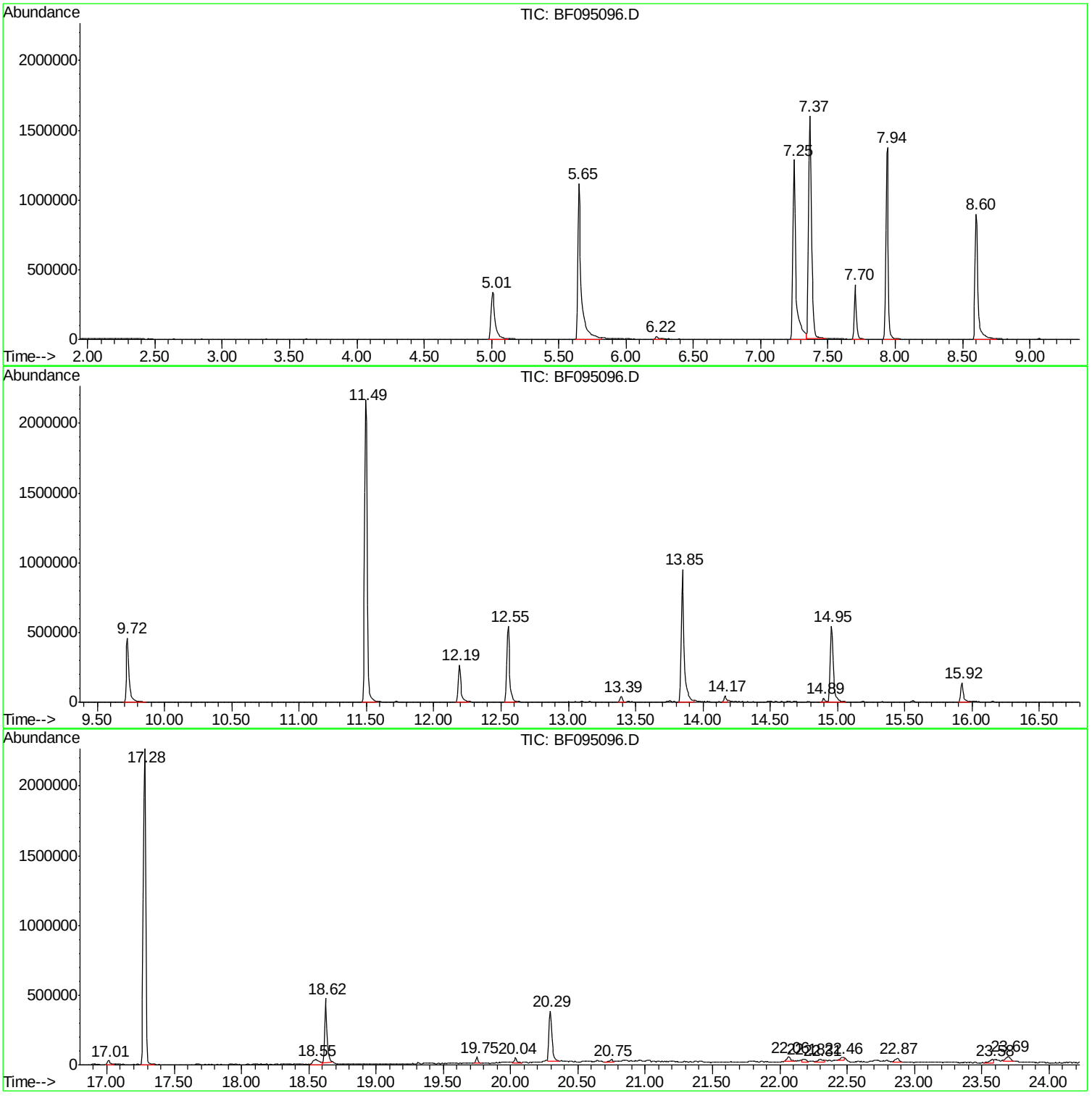
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051117\
Data File : BF095096.D
Acq On : 11 May 2017 23:53
Operator : SJ/MA
Sample : I3087-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01_001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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\BF051117\
Data File : BF095096.D
Acq On : 11 May 2017 23:53
Operator : SJ/MA
Sample : I3087-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01_001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

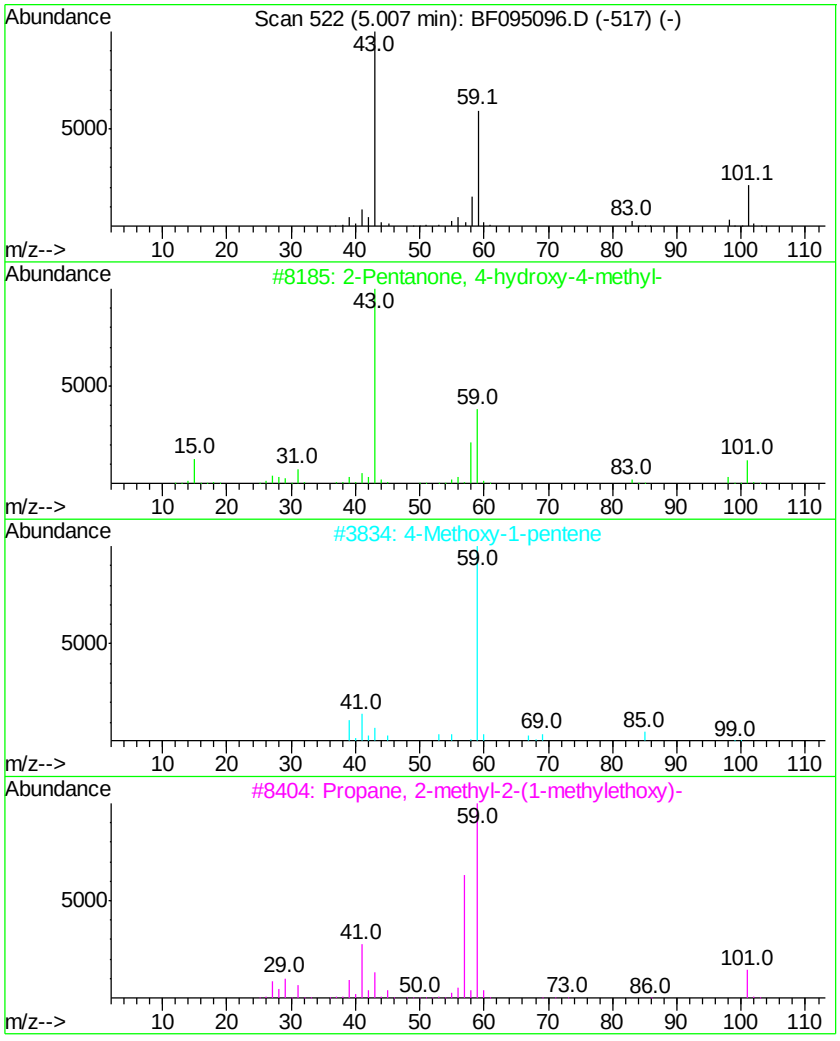
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

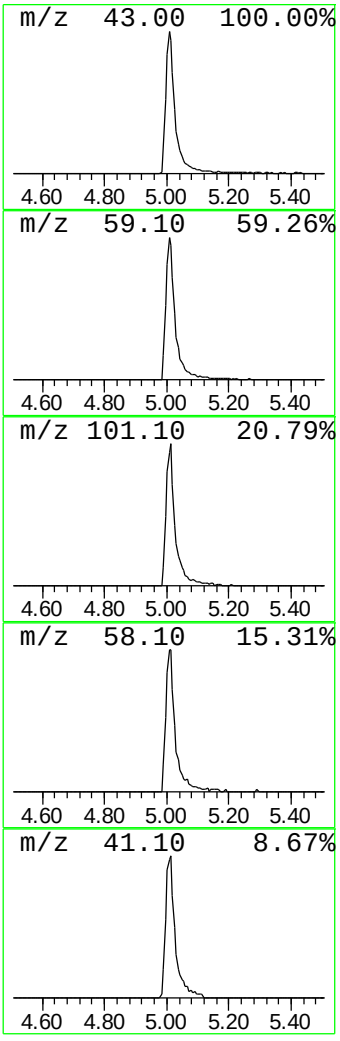
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	30.21 ng	708458	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	4-Methoxy-1-pentene	100	C6H12O	098386-09-5	35
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF051117\
Data File : BF095096.D
Acq On : 11 May 2017 23:53
Operator : SJ/MA
Sample : I3087-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01_001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

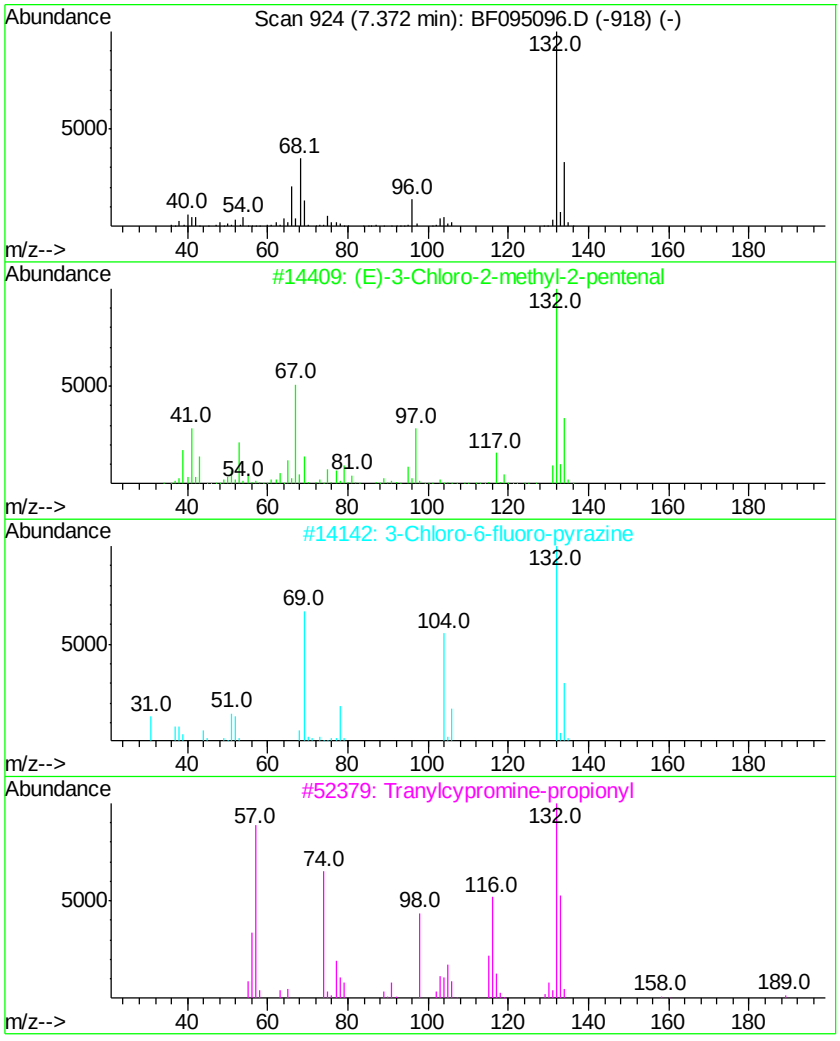
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

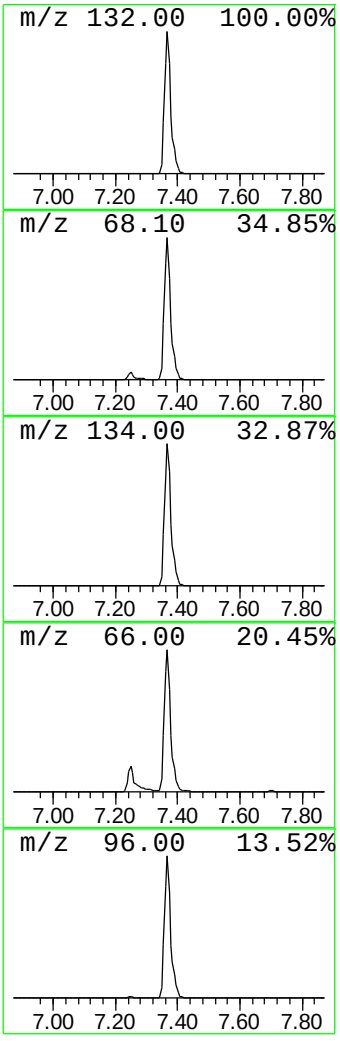
****

Peak Number 2 unknown7.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.37	98.70 ng	2314530	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF051117\
Data File : BF095096.D
Acq On : 11 May 2017 23:53
Operator : SJ/MA
Sample : I3087-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01_001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

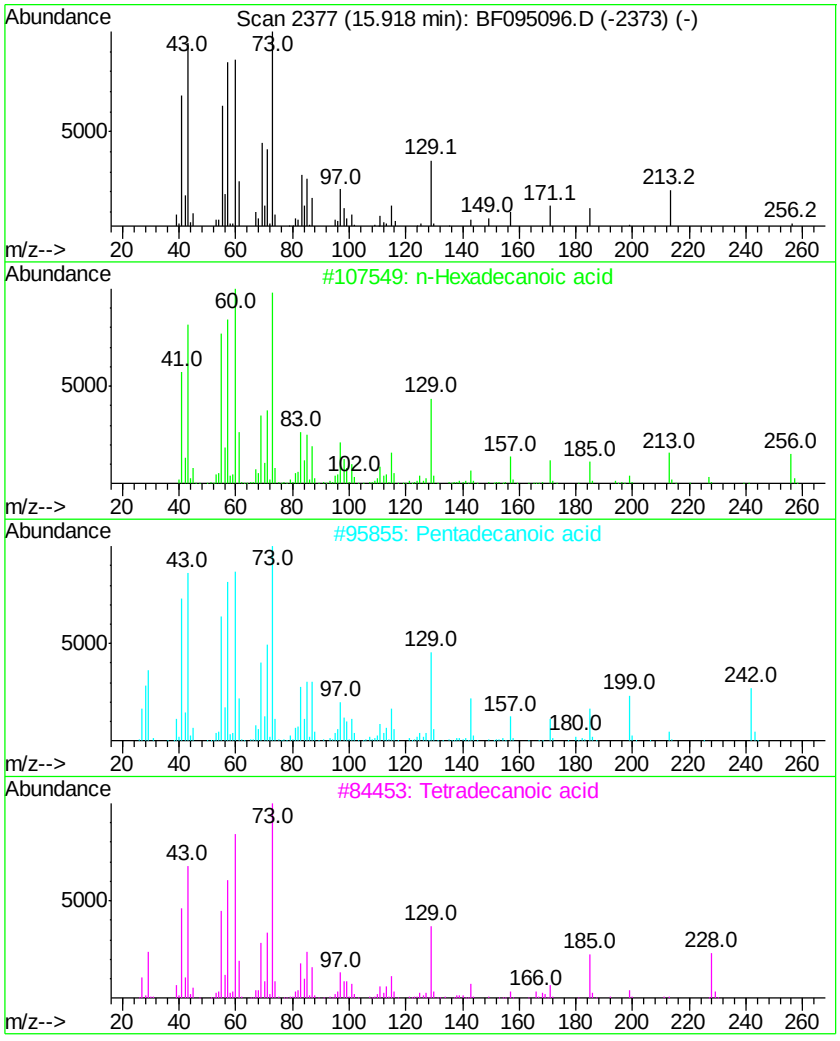
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

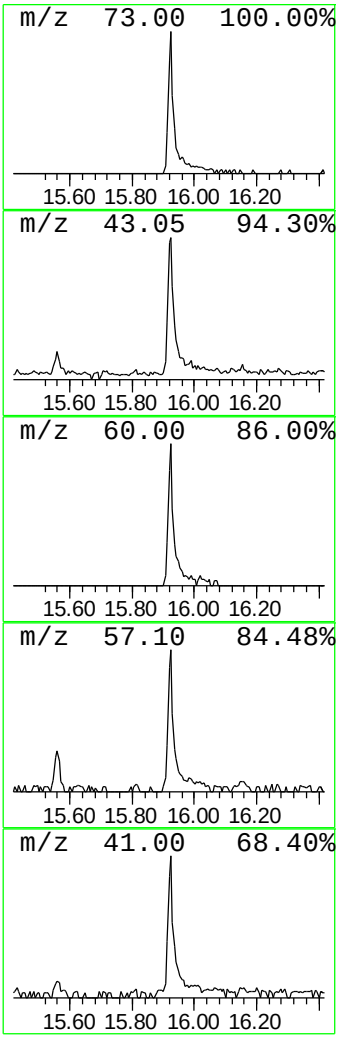
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.92	4.45 ng	179900	Phenanthrene-d10	14.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051117\
Data File : BF095096.D
Acq On : 11 May 2017 23:53
Operator : SJ/MA
Sample : I3087-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01_001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

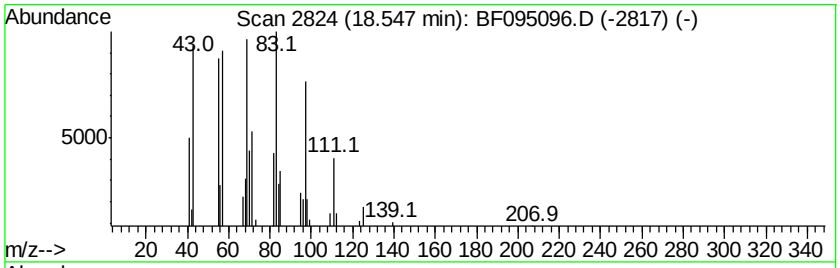
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

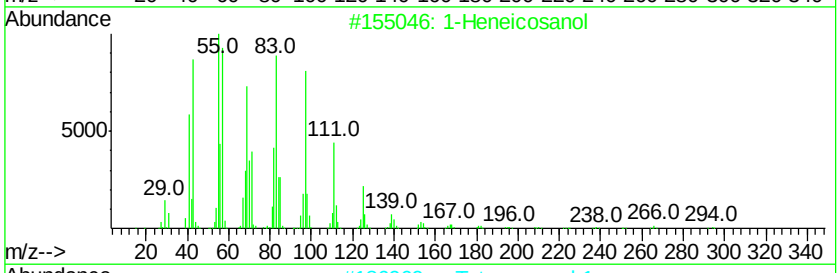
****

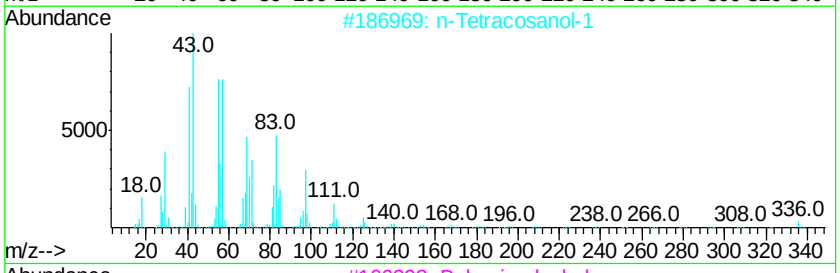
Peak Number 5 1-Heneicosanol Concentration Rank 5

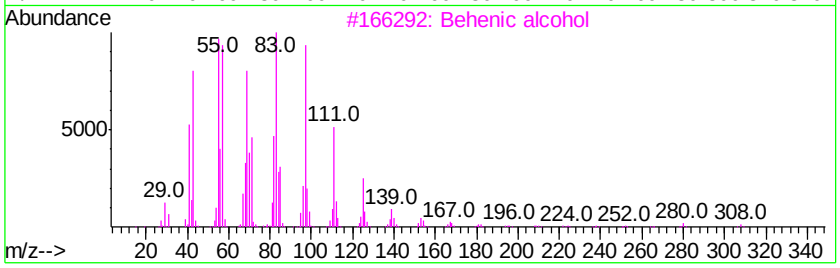
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.55	4.00 ng	121340	Chrysene-d12	18.62

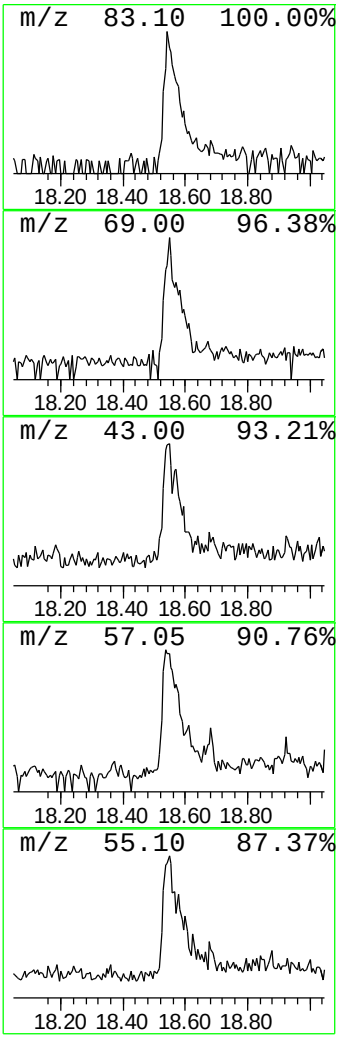
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	91
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
5	1-Hexadecanol	242	C16H34O	036653-82-4	90











Data Path : Z:\HPCHEM1\BNA F\DATA\BF051117\
Data File : BF095096.D
Acq On : 11 May 2017 23:53
Operator : SJ/MA
Sample : I3087-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01_001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

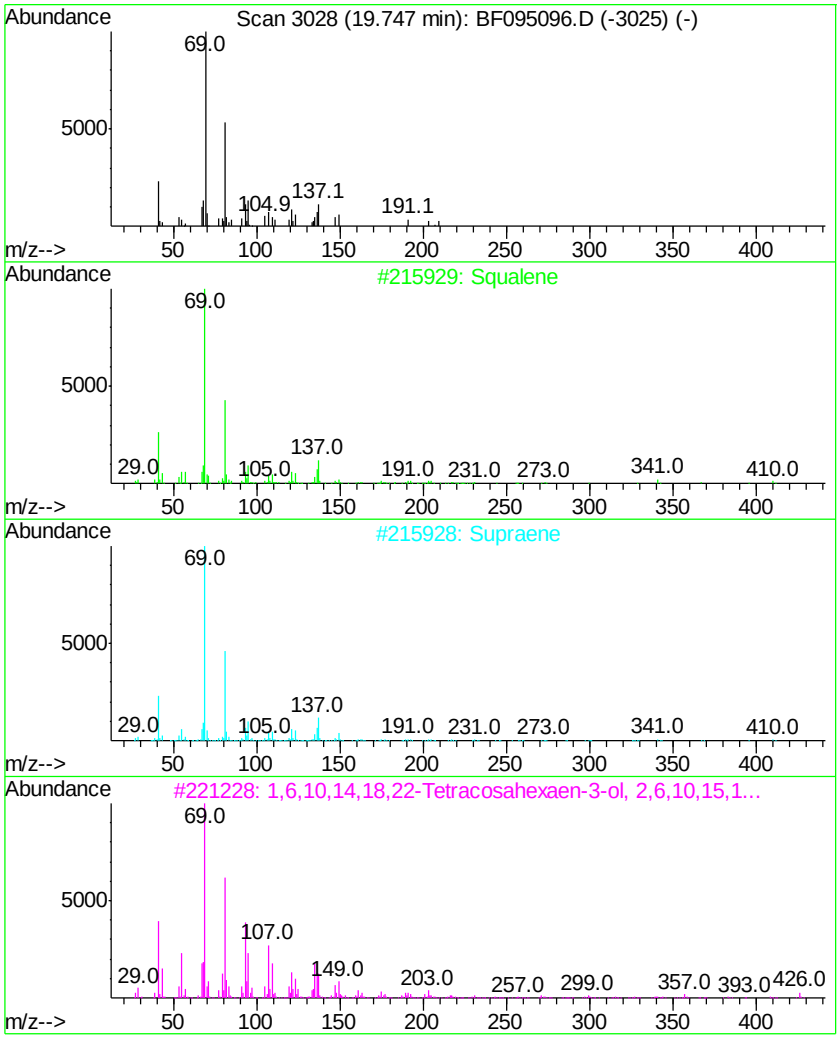
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

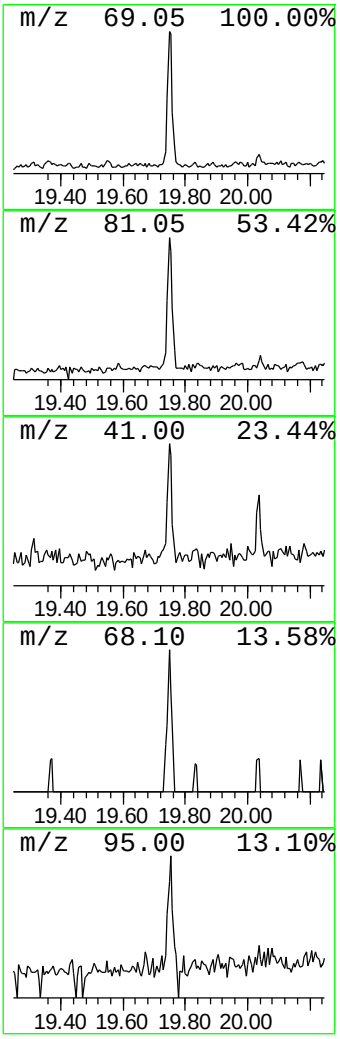
****

Peak Number 6 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.75	2.10 ng	53551	Perylene-d12	20.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	78
2	Supraene	410	C30H50	007683-64-9	72
3	1,6,10,14,18,22-Tetracosahexaen-...	426	C30H50O	054159-46-5	72
4	Propanoic acid, 2,2-dimethyl-, [...	306	C20H34O2	1000164-38-8	53
5	2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	50





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051117\
Data File : BF095096.D
Acq On : 11 May 2017 23:53
Operator : SJ/MA
Sample : I3087-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01_001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

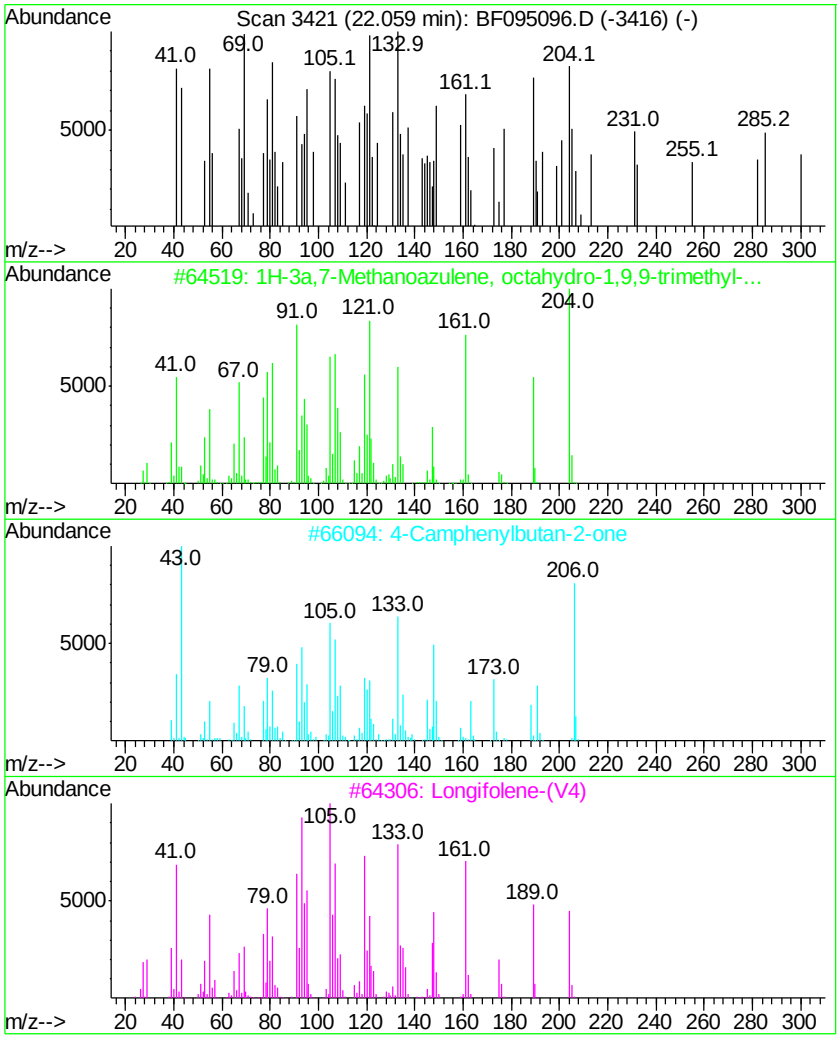
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

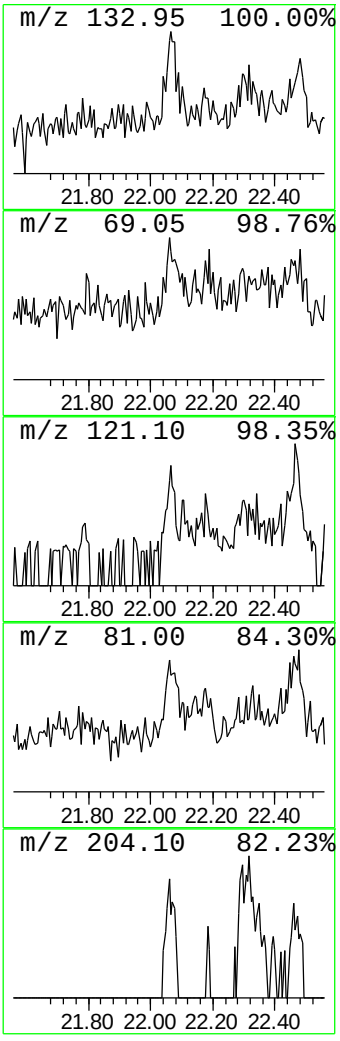
****

Peak Number 7 1H-3a,7-Methanoazulene, oct... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.06	2.96 ng	75435	Perylene-d12	20.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	55
2	4-Camphenylbutan-2-one	206	C14H22O	1000140-09-7	40
3	Longifolene-(V4)	204	C15H24	061262-67-7	38
4	Longifolene	204	C15H24	000475-20-7	35
5	.alpha.-Guaiene	204	C15H24	003691-12-1	30





Data Path : Z:\HPCHEM1\BNA F\DATA\BF051117\
Data File : BF095096.D
Acq On : 11 May 2017 23:53
Operator : SJ/MA
Sample : I3087-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01_001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

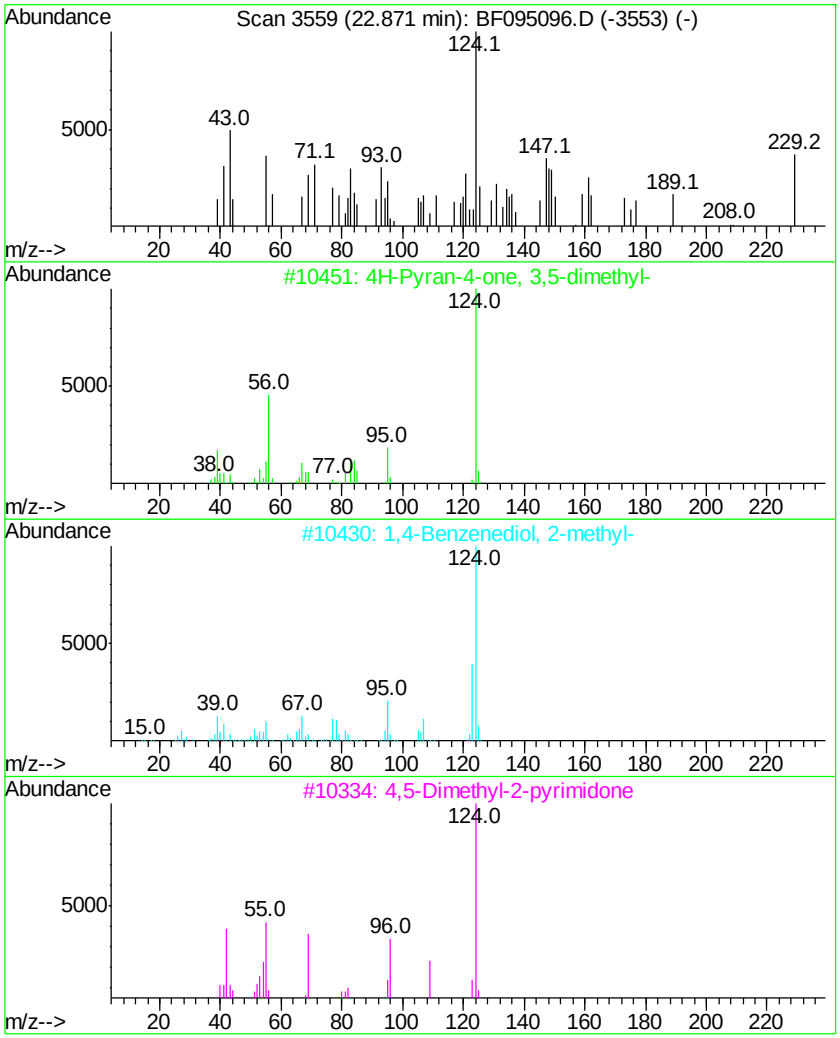
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

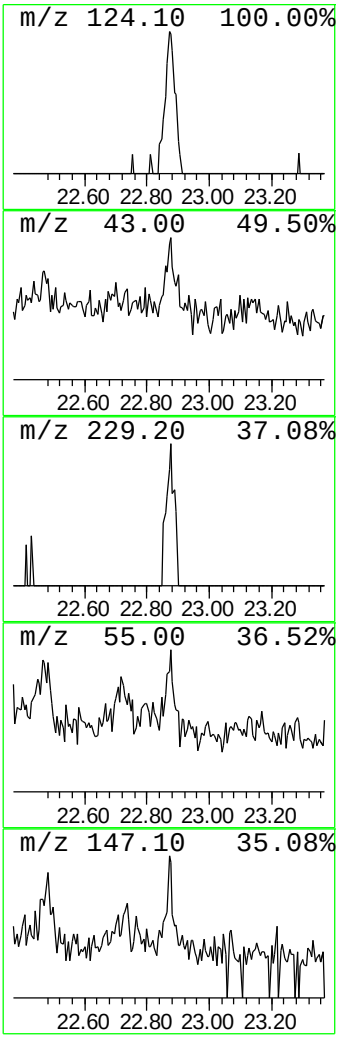
****

Peak Number 8 unknown22.87 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.87	2.47 ng	63071	Perylene-d12	20.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Pyran-4-one, 3,5-dimethyl-	124	C7H8O2	019083-61-5	27
2	1,4-Benzenediol, 2-methyl-	124	C7H8O2	000095-71-6	27
3	4,5-Dimethyl-2-pyrimidone	124	C6H8N2O	034939-17-8	22
4	2,4-Diaminophenol	124	C6H8N2O	000095-86-3	16
5	1,3-Benzenediol, 2-methyl-	124	C7H8O2	000608-25-3	16





Data Path : Z:\HPCHEM1\BNA F\DATA\BF051117\
Data File : BF095096.D
Acq On : 11 May 2017 23:53
Operator : SJ/MA
Sample : I3087-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01_001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

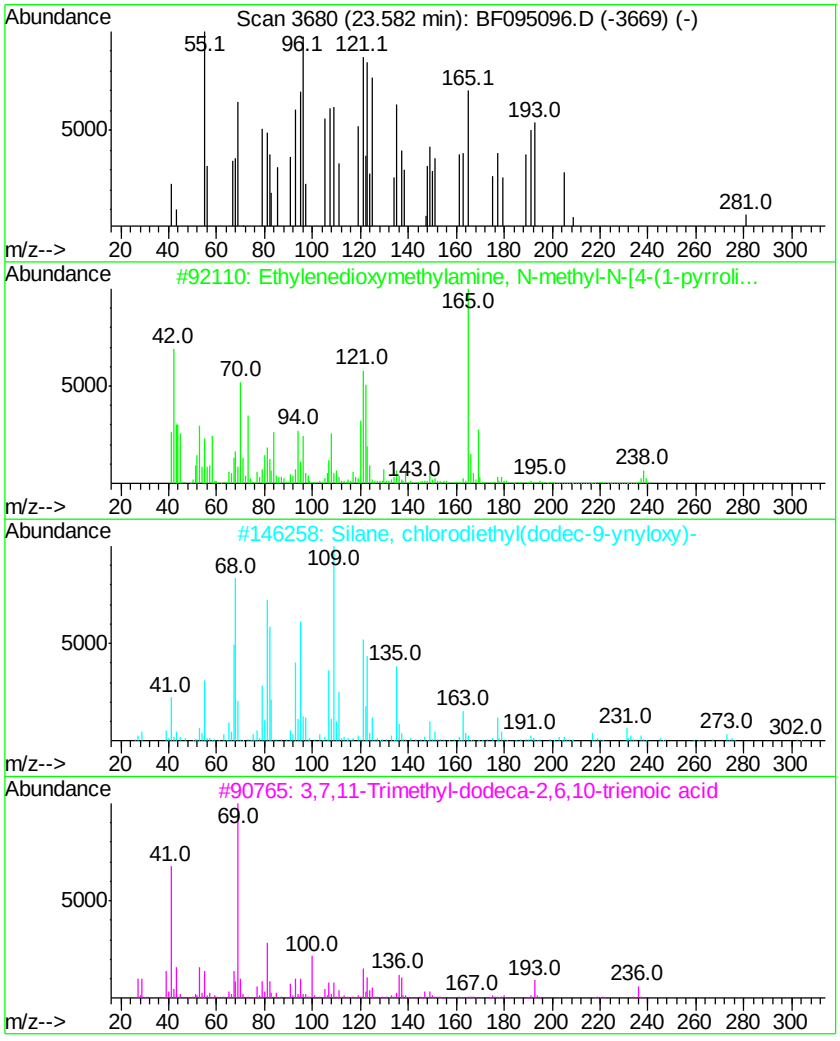
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

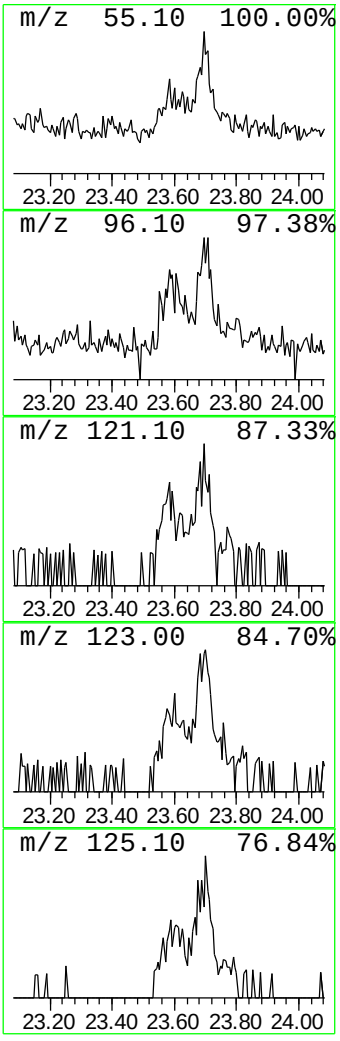
****

Peak Number 9 unknown23.58 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.58	2.14 ng	54555	Perylene-d12	20.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethylenedioxymethylamine, N-meth...	238	C13H22N2O2	153817-36-8	27
2	Silane, chlorodiethyl(dodec-9-yn...	302	C16H31ClOSi	1000363-59-2	25
3	3,7,11-Trimethyl-dodeca-2,6,10-t...	236	C15H24O2	007548-13-2	16
4	2-Hydroxy-6-methyl-6,7-dihydro-9...	193	C10H11NO3	1000210-15-9	11
5	1-(2-Pyridyl)piperazine	163	C9H13N3	034803-66-2	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF051117\
Data File : BF095096.D
Acq On : 11 May 2017 23:53
Operator : SJ/MA
Sample : I3087-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01_001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

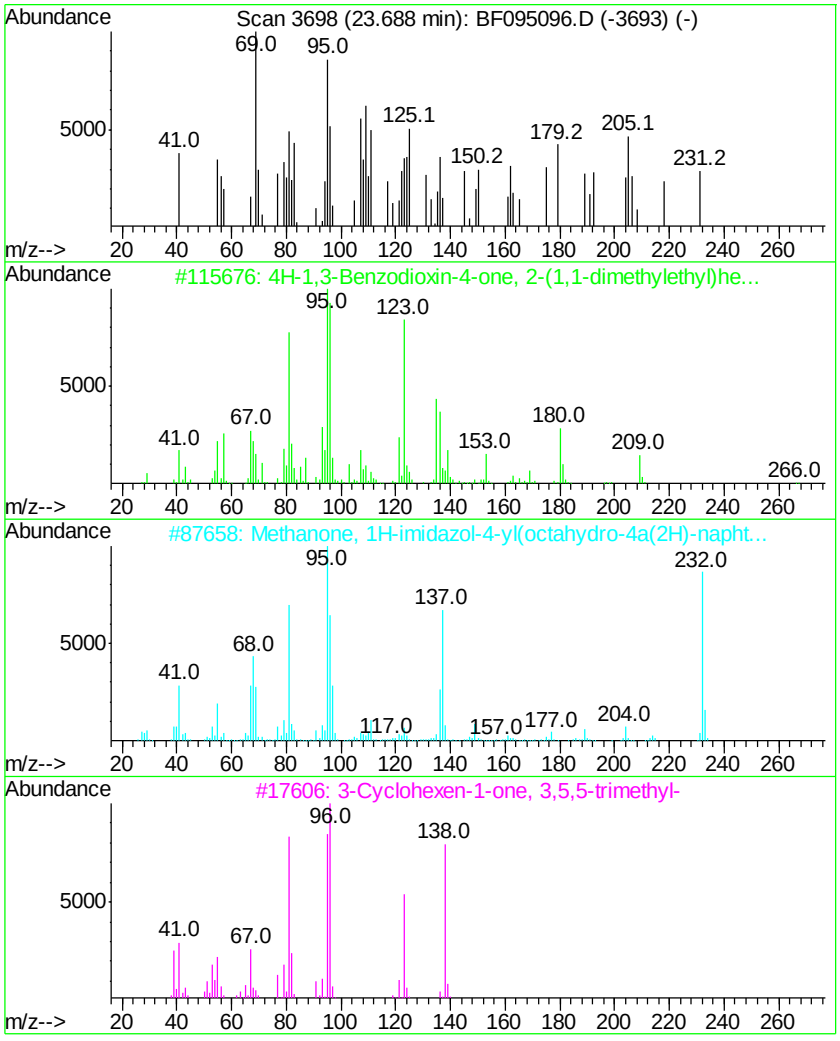
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

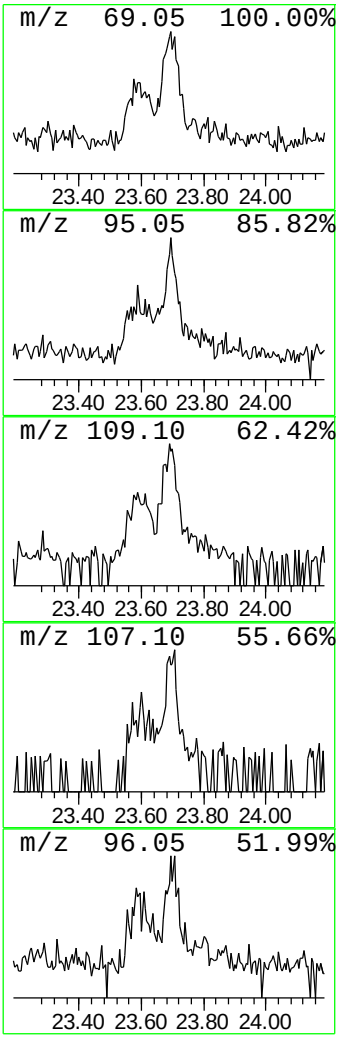
****

Peak Number 10 unknown23.69 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.69	3.61 ng	92123	Perylene-d12	20.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-1,3-Benzodioxin-4-one, 2-(1,1...	266	C16H26O3	124899-18-9	35
2	Methanone, 1H-imidazol-4-yl(octa...	232	C14H20N2O	069393-47-1	35
3	3-Cyclohexen-1-one, 3,5,5-trimet...	138	C9H14O	000471-01-2	18
4	2(1H)-Naphthalenone, 4a,5,6,7,8,...	220	C15H24O	017408-66-1	15
5	Longifolenaldehyde	220	C15H24O	019890-84-7	15





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051117\
Data File : BF095096.D
Acq On : 11 May 2017 23:53
Operator : SJ/MA
Sample : I3087-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01_001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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...	5.01	30.2	ng	708458	1	7.70	469019	20.0
unknown7.37	7.37	98.7	ng	2314530	1	7.70	469019	20.0
n-Hexadecanoic acid	15.92	4.5	ng	179900	4	14.95	808329	20.0
1-Heneicosanol	18.55	4.0	ng	121340	5	18.62	605957	20.0
Squalene	19.75	2.1	ng	53551	6	20.29	510419	20.0
1H-3a,7-Methanoaz...	22.06	3.0	ng	75435	6	20.29	510419	20.0
unknown22.87	22.87	2.5	ng	63071	6	20.29	510419	20.0
unknown23.58	23.58	2.1	ng	54555	6	20.29	510419	20.0
unknown23.69	23.69	3.6	ng	92123	6	20.29	510419	20.0