LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF021416\
Data File : BF085076.D
Acq On : 13 Feb 2016 10:16
Operator : SJ/IZ
Sample : H1409-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B039(9-11)

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-BF021316.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	1.678	6	8	10	rVB	148719	189909	2.94%	0.384%
2	1.724	10	12	50	rVB	1398650	4677870	72.35%	9.468%
3	3.701	183	185	199	rBV	230011	783554	12.12%	1.586%
4	4.136	220	223	249	rBV	730865	3685271	57.00%	7.459%
5	5.427	333	336	341	rBV	662421	2216233	34.28%	4.486%
6	5.564	345	348	374	rVV	1478548	6465239	100.00%	13.086%
7	5.907	374	378	391	rVV	153399	1185292	18.33%	2.399%
8	6.090	391	394	436	rVB	962220	3868603	59.84%	7.830%
9	6.719	446	449	478	rBV	434056	2887160	44.66%	5.844%
10	7.793	540	543	577	rBV	153553	1137006	17.59%	2.301%
11	9.530	692	695	737	rBV	1447285	4823533	74.61%	9.763%
12	10.216	752	755	774	rBV	117451	560830	8.67%	1.135%
13	10.582	784	787	806	rBV	394075	1387864	21.47%	2.809%
14	11.416	857	860	870	rBV	47808	140716	2.18%	0.285%
15	11.885	897	901	925	rVV	772854	3353430	51.87%	6.788%
16	12.194	925	928	940	rVB2	58998	201575	3.12%	0.408%
17	13.005	995	999	1017	rVB	288796	1132729	17.52%	2.293%
18	14.925	1164	1167	1180	rVV	551942	888933	13.75%	1.799%
19	15.542	1218	1221	1225	rVV	81183	146441	2.27%	0.296%
20	15.622	1225	1228	1247	rVB	1590009	3518579	54.42%	7.122%
21	16.125	1269	1272	1279	rBV	850772	1244061	19.24%	2.518%
22	16.308	1284	1288	1292	rVB2	50033	95513	1.48%	0.193%
23	16.628	1314	1316	1317	rBV	45479	86470	1.34%	0.175%
24	17.108	1354	1358	1362	rBV	524303	1004521	15.54%	2.033%
25	17.177	1362	1364	1377	rVB	402931	907195	14.03%	1.836%
26	17.897	1423	1427	1431	rBV	154183	311894	4.82%	0.631%
27	18.583	1482	1487	1497	rBV2	158654	396536	6.13%	0.803%
28	18.800	1503	1506	1513	rBV	344254	771371	11.93%	1.561%
29	19.314	1549	1551	1564	rVV	205737	604082	9.34%	1.223%
30	19.737	1586	1588	1599	rVB	26867	92535	1.43%	0.187%
31	20.274	1632	1635	1641	rBV5	26487	98861	1.53%	0.200%
32	20.594	1658	1663	1669	rBV	154605	399575	6.18%	0.809%
33	20.812	1679	1682	1687	rVB5	28589	76135	1.18%	0.154%
34	21.303	1721	1725	1728	rBV4	27635	66413	1.03%	0.134%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF021416\
Data File : BF085076.D
Acq On : 13 Feb 2016 10:16
Operator : SJ/IZ
Sample : H1409-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B039(9-11)

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-BF021316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

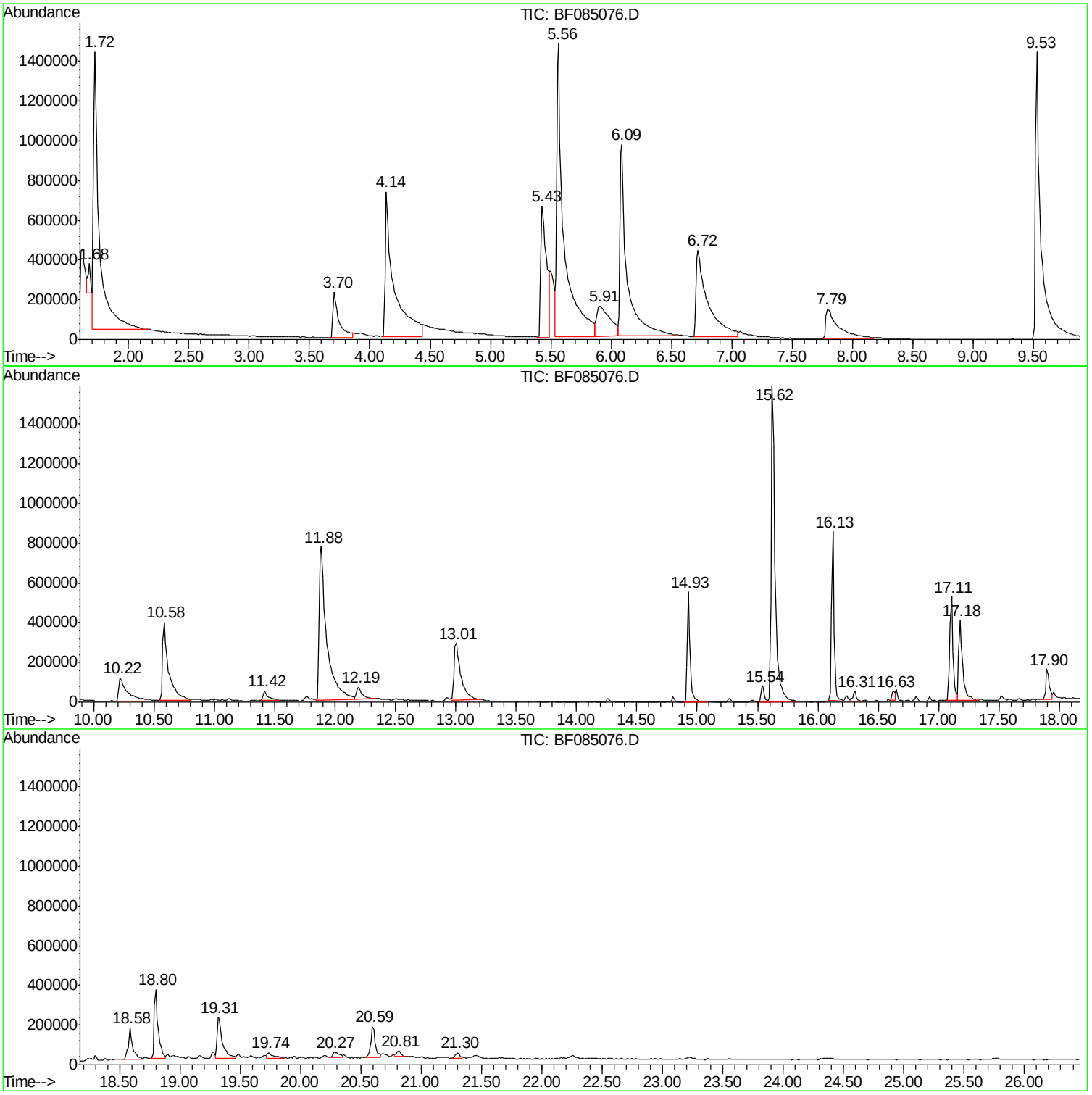
Sum of corrected areas: 49405929

Data Path : Z:\HPCHEM1\BNA F\DATA\BF021416\
Data File : BF085076.D
Acq On : 13 Feb 2016 10:16
Operator : SJ/IZ
Sample : H1409-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B039(9-11)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021316.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\BF021416\
Data File : BF085076.D
Acq On : 13 Feb 2016 10:16
Operator : SJ/IZ
Sample : H1409-08
Misc :
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Instrument : BNA_F
ClientSampleId : SUP-B039(9-11)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

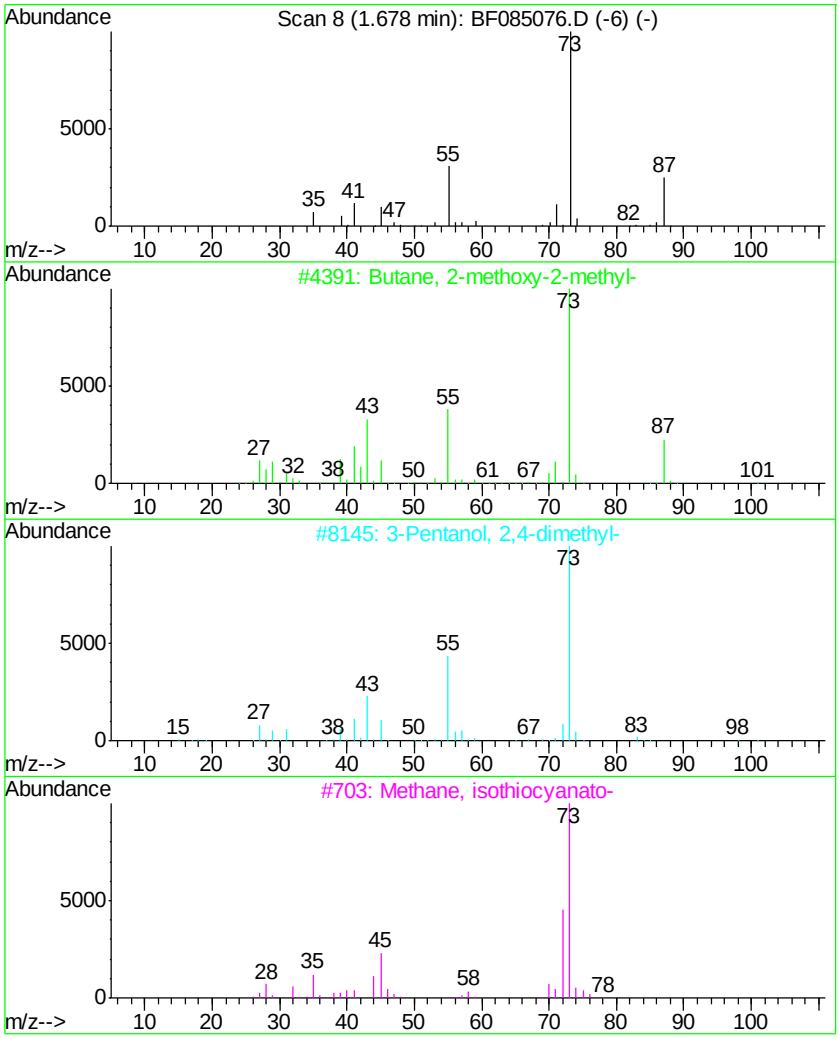
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

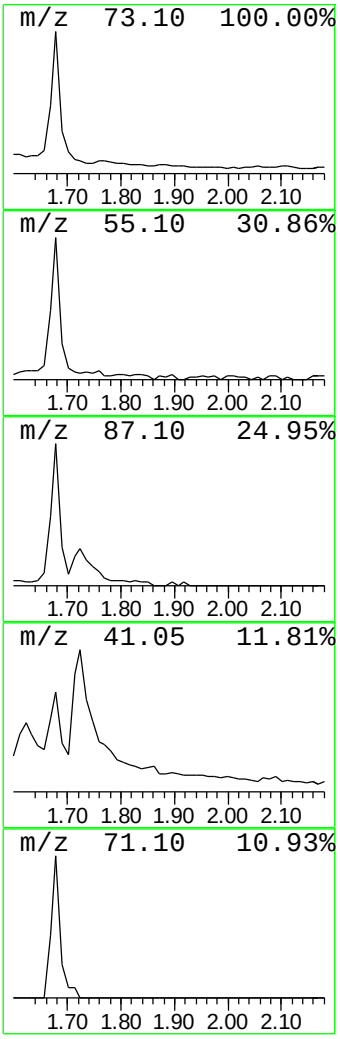
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.68	3.20 ng	189909	1,4-Dichlorobenzene-d4	5.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	17
3	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF021416\
Data File : BF085076.D
Acq On : 13 Feb 2016 10:16
Operator : SJ/IZ
Sample : H1409-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B039(9-11)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

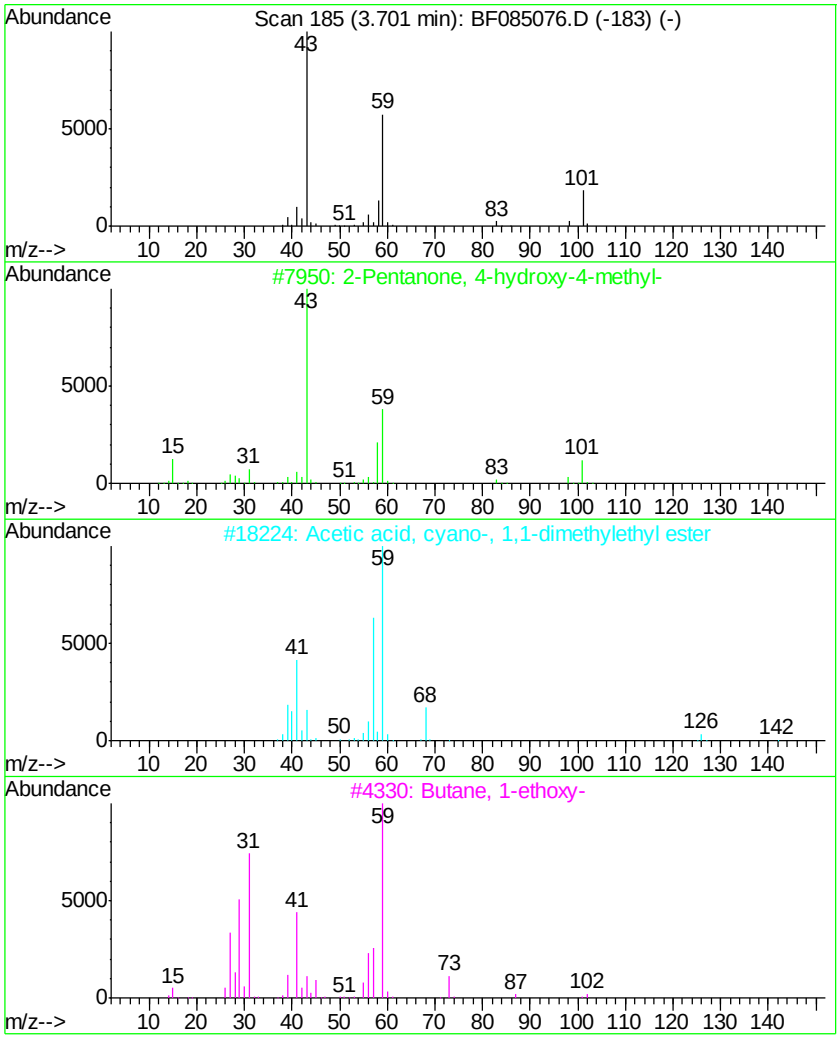
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

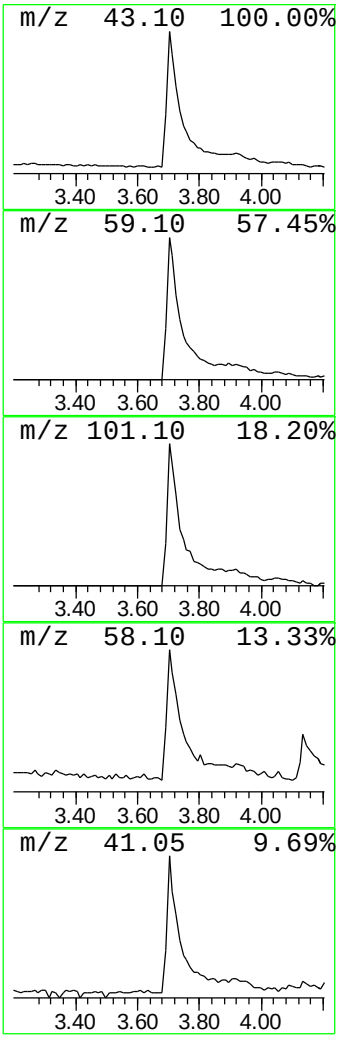
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.70	13.22 ng	783554	1,4-Dichlorobenzene-d4	5.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF021416\
Data File : BF085076.D
Acq On : 13 Feb 2016 10:16
Operator : SJ/IZ
Sample : H1409-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B039(9-11)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

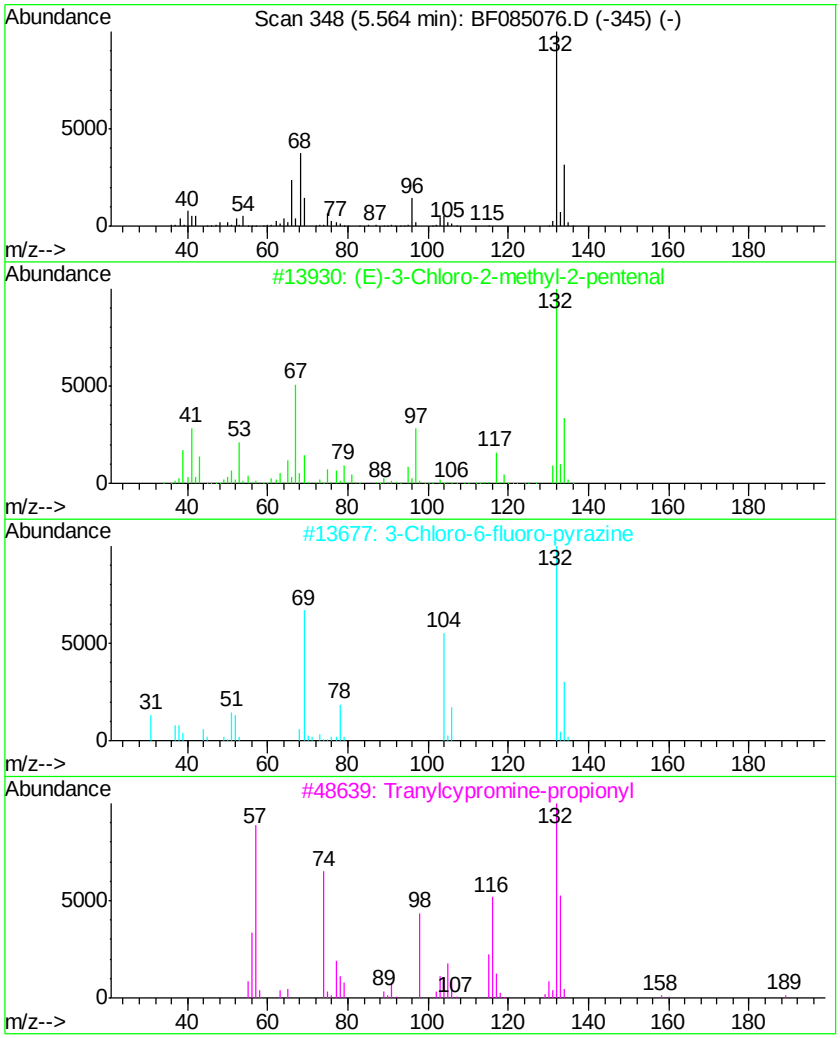
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

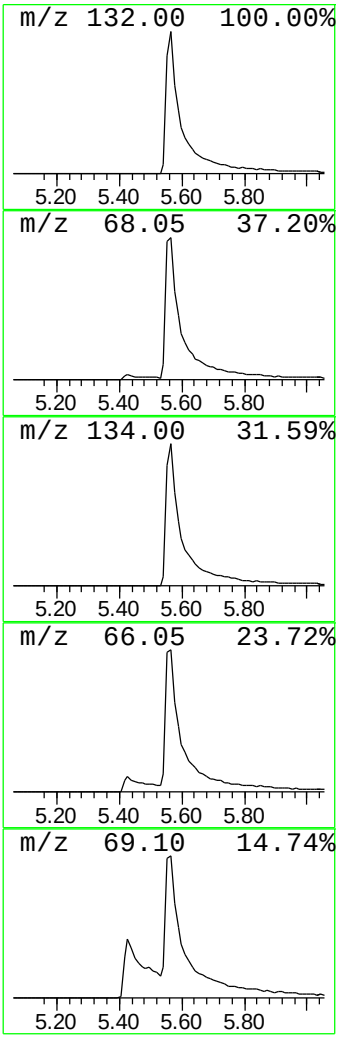
****

Peak Number 4 unknown5.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.56	109.09 ng	6465240	1,4-Dichlorobenzene-d4	5.91

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	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	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\BF021416\
Data File : BF085076.D
Acq On : 13 Feb 2016 10:16
Operator : SJ/IZ
Sample : H1409-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B039(9-11)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

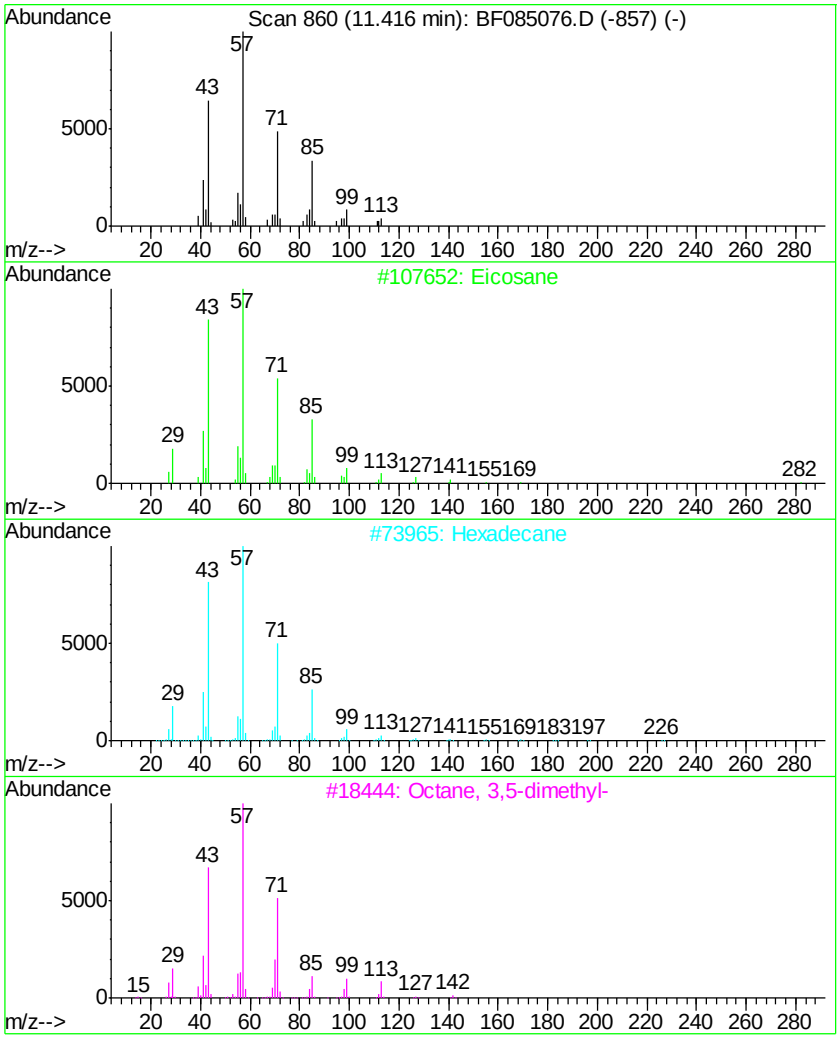
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

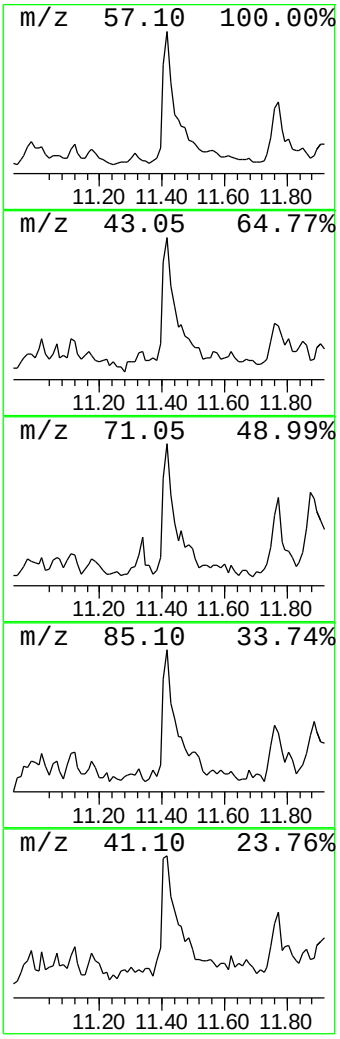
****

Peak Number 6 Eicosane Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.42	2.03 ng	140716	Acenaphthene-d10	10.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	86
2	Hexadecane	226	C16H34	000544-76-3	83
3	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	64
4	Tetradecane	198	C14H30	000629-59-4	64
5	Tridecane	184	C13H28	000629-50-5	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF021416\
Data File : BF085076.D
Acq On : 13 Feb 2016 10:16
Operator : SJ/IZ
Sample : H1409-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B039(9-11)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

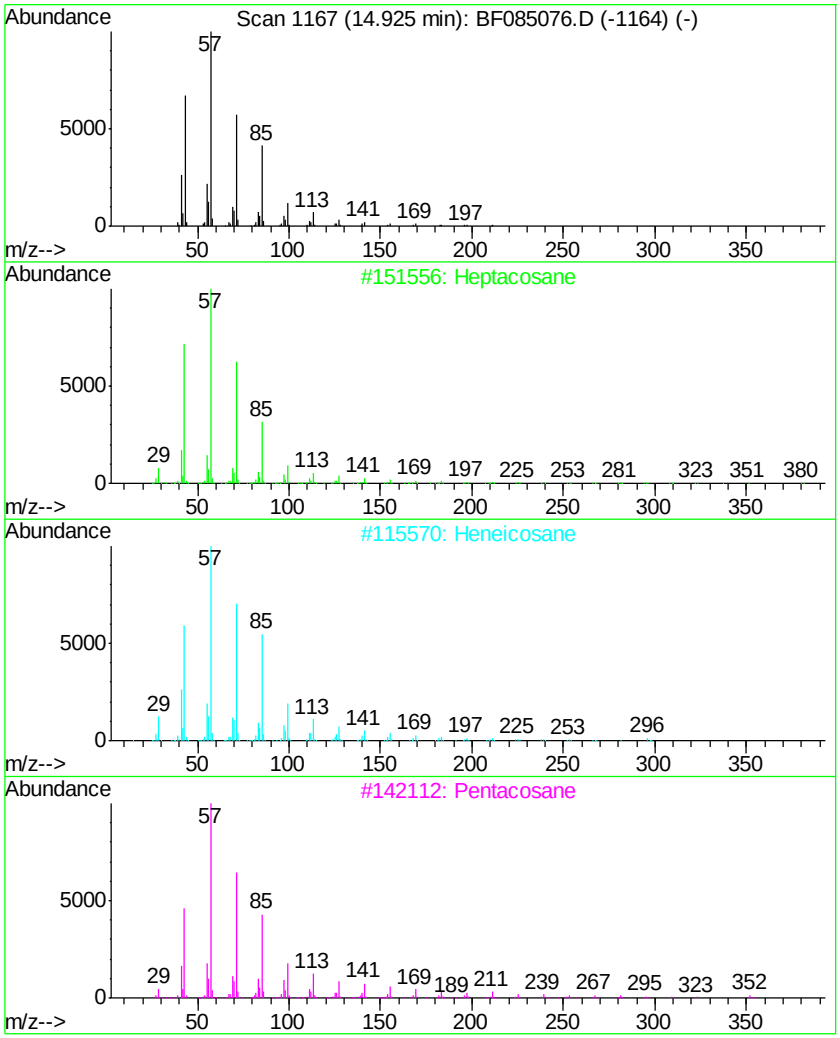
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

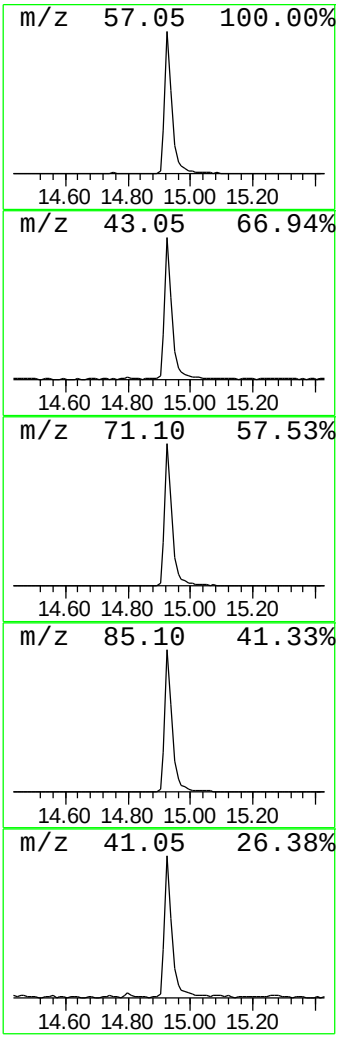
****

Peak Number 8 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	15.70 ng	888933	Phenanthrene-d10	13.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	Pentacosane	352	C25H52	000629-99-2	90
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF021416\
Data File : BF085076.D
Acq On : 13 Feb 2016 10:16
Operator : SJ/IZ
Sample : H1409-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B039(9-11)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

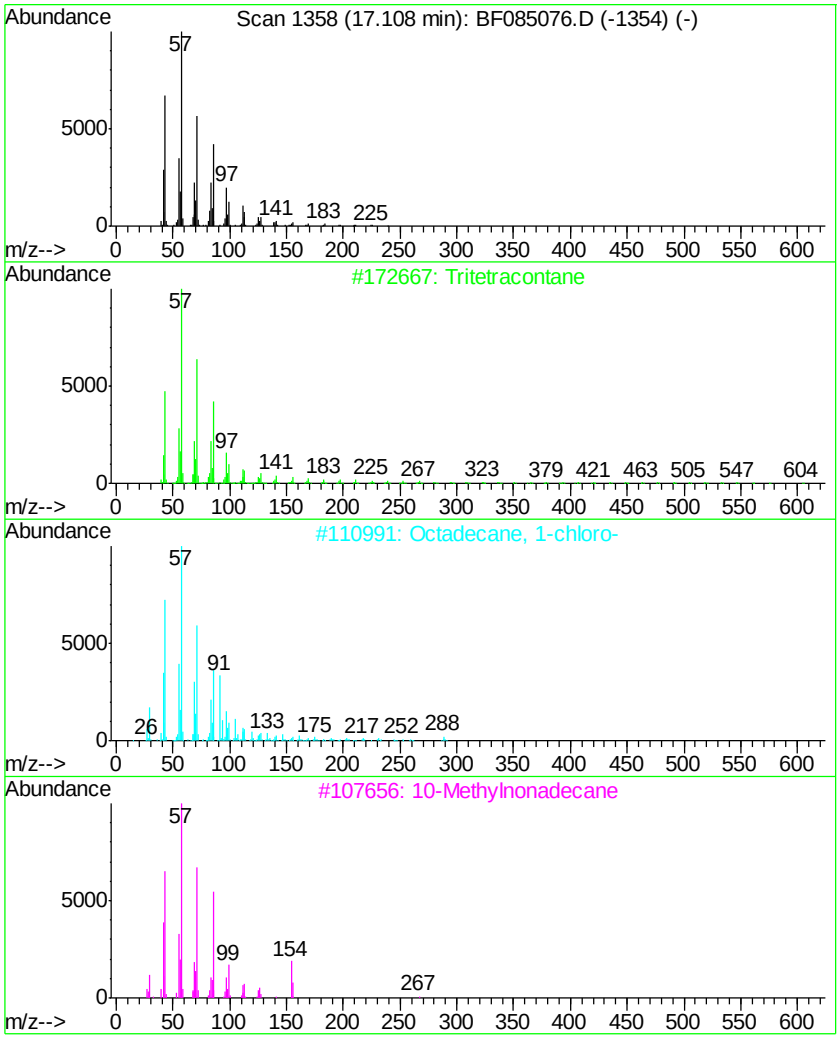
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

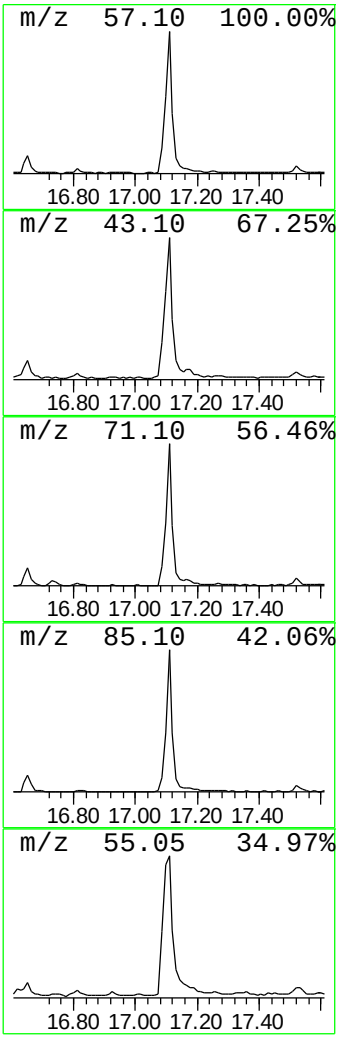
****

Peak Number 12 Tritetracontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.11	22.15 ng	1004520	Chrysene-d12	17.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tritetracontane	605	C43H88	007098-21-7	91
2	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	91
3	10-Methylnonadecane	282	C20H42	056862-62-5	72
4	Tetradecane	198	C14H30	000629-59-4	62
5	Nonadecane	268	C19H40	000629-92-5	62





Data Path : Z:\HPCHEM1\BNA F\DATA\BF021416\
Data File : BF085076.D
Acq On : 13 Feb 2016 10:16
Operator : SJ/IZ
Sample : H1409-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B039(9-11)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

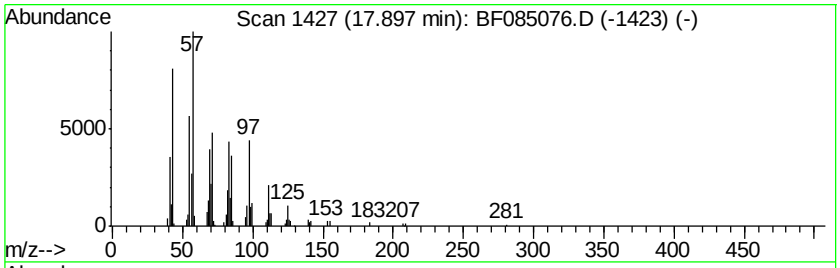
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

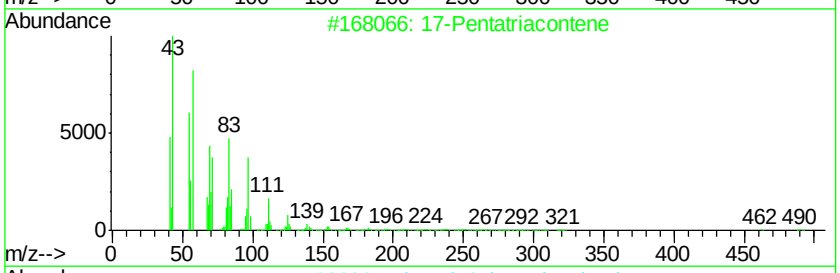
****

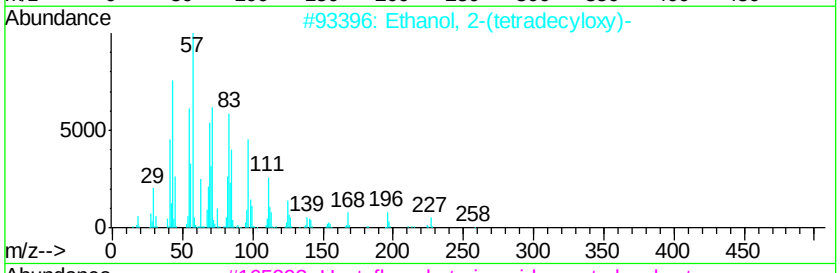
Peak Number 13 17-Pentatriacontene Concentration Rank 11

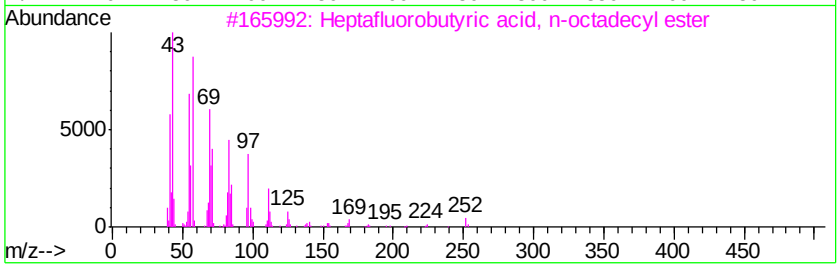
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.90	6.88 ng	311894	Chrysene-d12	17.18

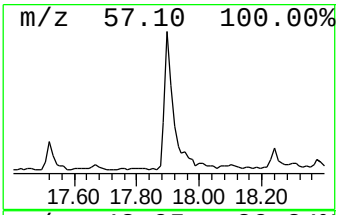
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	91
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	87
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	87
5	1-Docosene	308	C22H44	001599-67-3	81

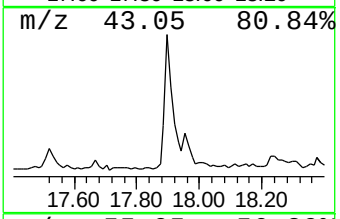


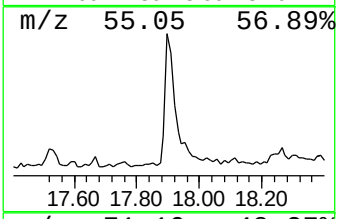


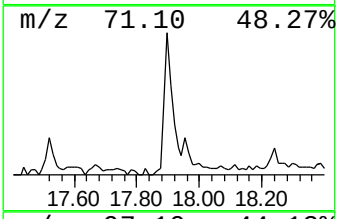


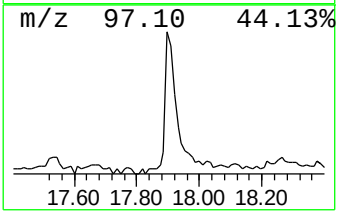












Data Path : Z:\HPCHEM1\BNA F\DATA\BF021416\
Data File : BF085076.D
Acq On : 13 Feb 2016 10:16
Operator : SJ/IZ
Sample : H1409-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B039(9-11)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

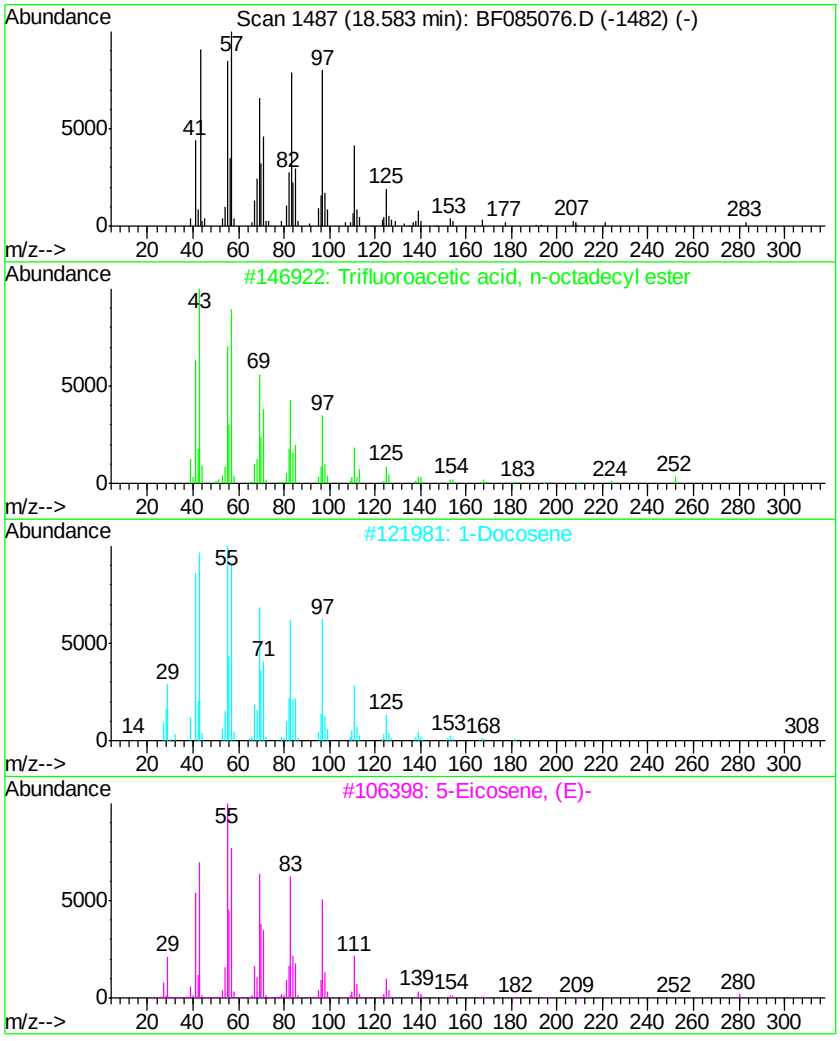
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

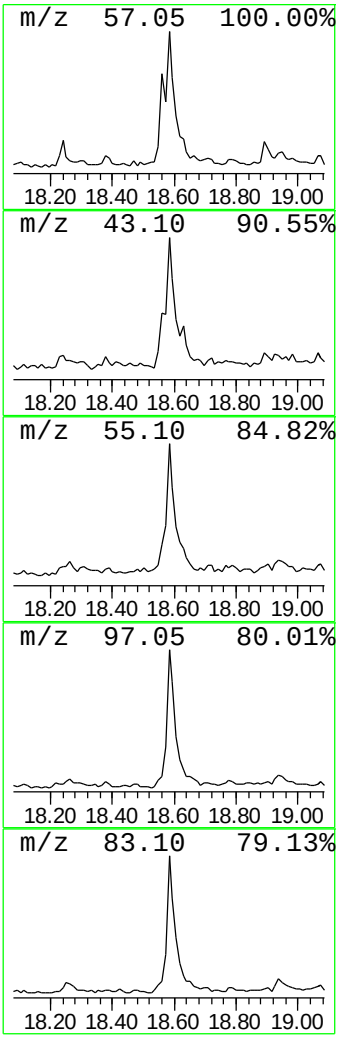
****

Peak Number 14 Trifluoroacetic acid, n-oct... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.58	10.28 ng	396536	Perylene-d12	18.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, n-octadecv...	366	C20H37F3O2	079392-43-1	91
2	1-Docosene	308	C22H44	001599-67-3	90
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	80
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	76
5	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	74





Data Path : Z:\HPCHEM1\BNA F\DATA\BF021416\
Data File : BF085076.D
Acq On : 13 Feb 2016 10:16
Operator : SJ/IZ
Sample : H1409-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B039(9-11)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

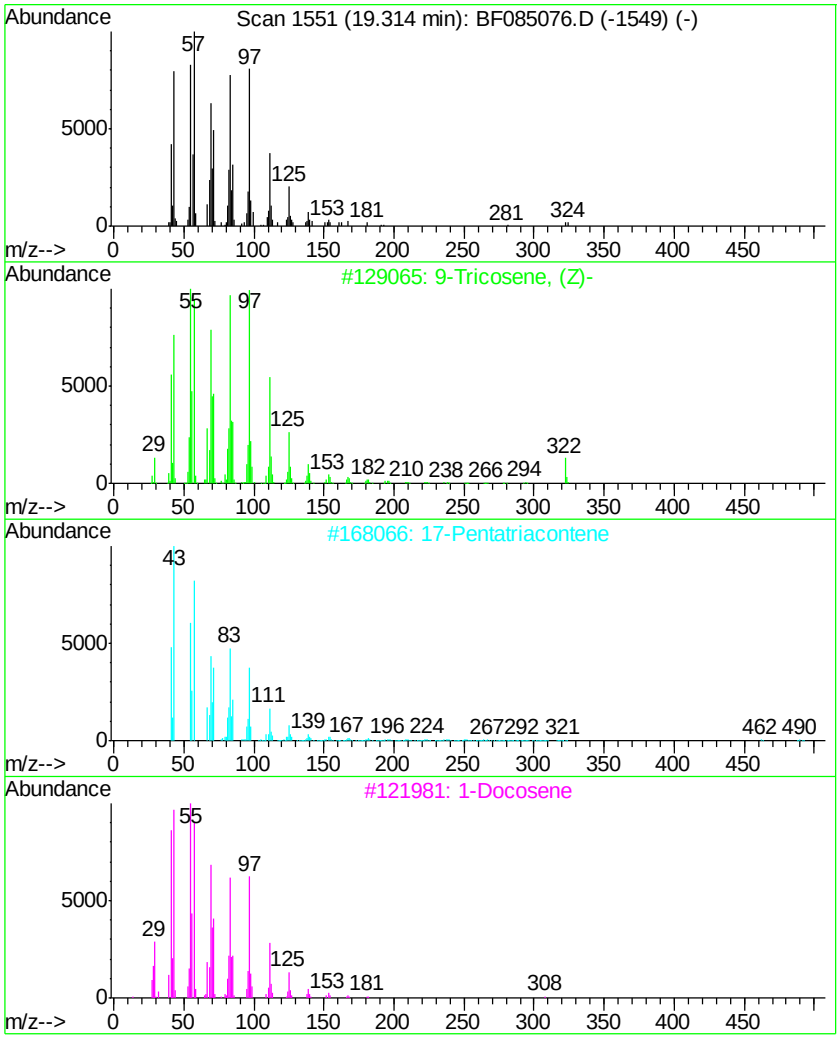
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

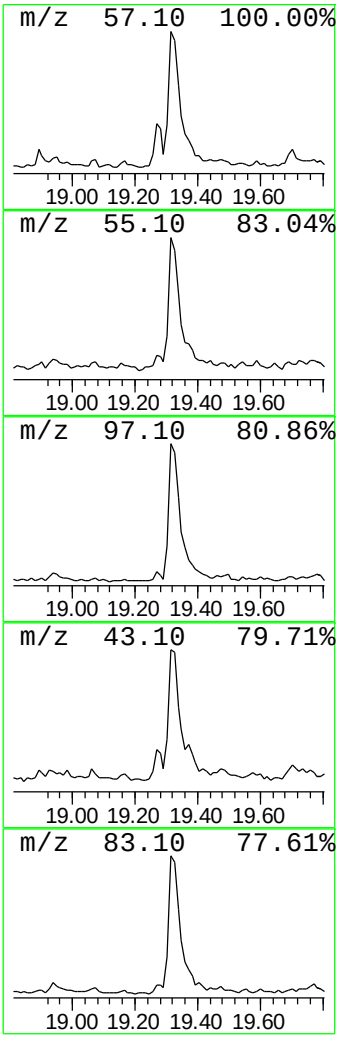
****

Peak Number 15 9-Tricosene, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.31	15.66 ng	604082	Perylene-d12	18.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Tricosene, (Z)-	322	C23H46	027519-02-4	93
2	17-Pentatriacontene	491	C35H70	006971-40-0	91
3	1-Docosene	308	C22H44	001599-67-3	87
4	1-Tricosene	322	C23H46	018835-32-0	86
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	81





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Acq On : 13 Feb 2016 10:16
Operator : SJ/IZ
Sample : H1409-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B039(9-11)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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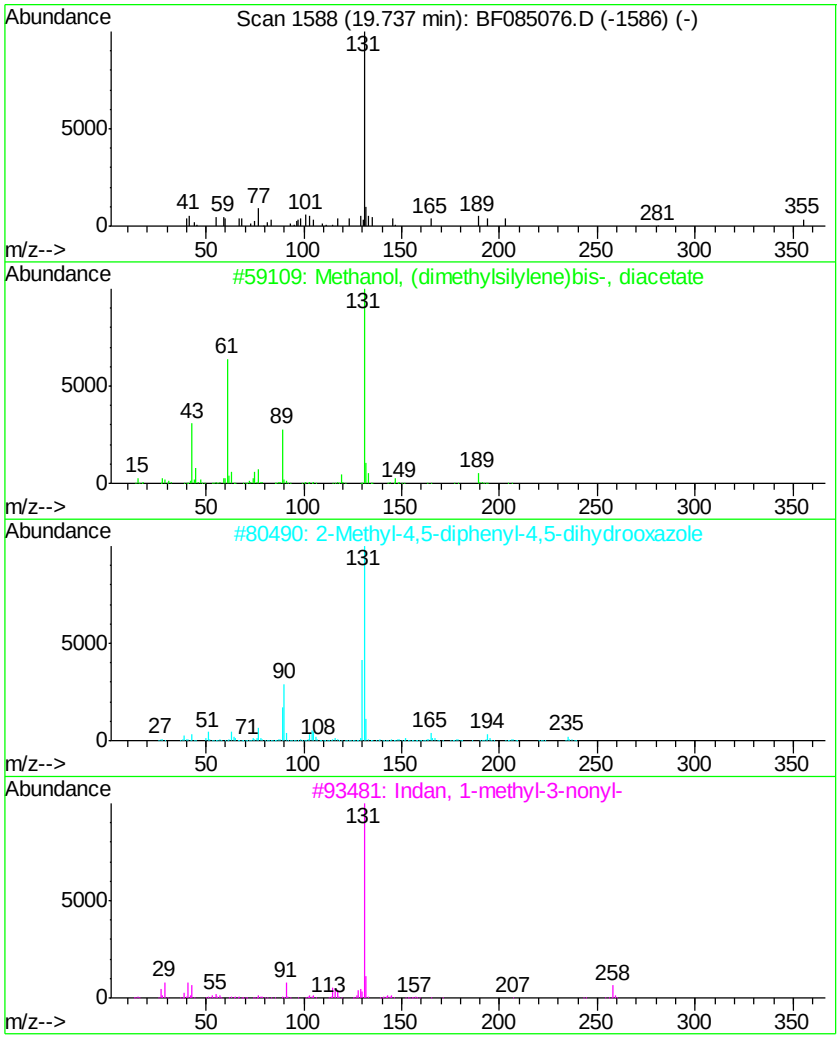
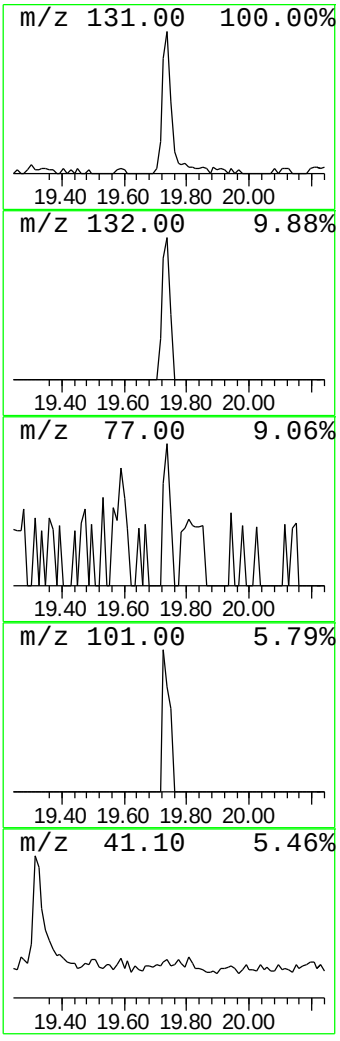
Peak Number 16 unknown19.74 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.74	2.40 ng	92535	Perylene-d12	18.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanol, (dimethylsilylene)bis-...	204	C8H16O4Si	002917-61-5	45
2	2-Methyl-4,5-diphenyl-4,5-dihydr...	237	C16H15NO	133649-09-9	45
3	Indan, 1-methyl-3-nonyl-	258	C19H30	029138-85-0	36
4	Naphthalene, 1,2,3,4-tetrahydro-...	258	C19H30	033425-49-9	36
5	Propanoic acid, dimethyl(isoprop...	174	C8H18O2Si	1000279-45-8	36





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Data File : BF085076.D
Acq On : 13 Feb 2016 10:16
Operator : SJ/IZ
Sample : H1409-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B039(9-11)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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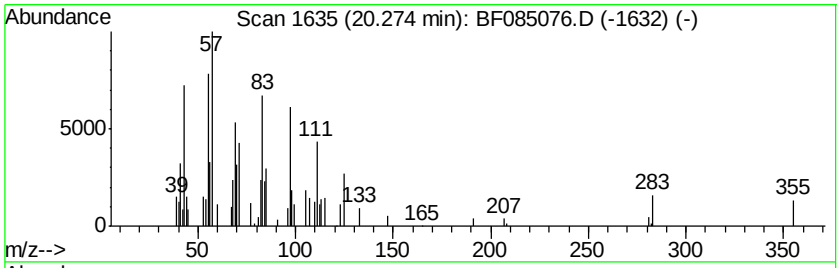
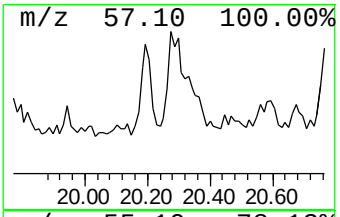
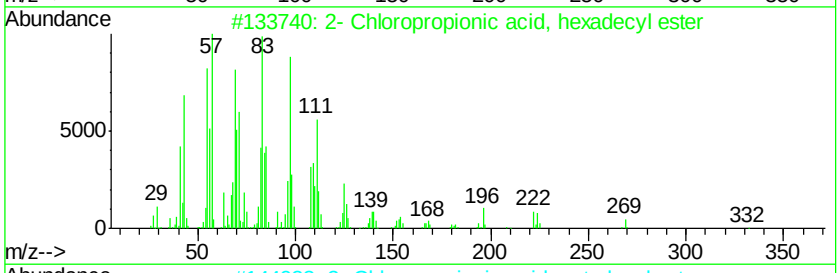
Peak Number 17 2- Chloropropionic acid, he... Concentration Rank 15

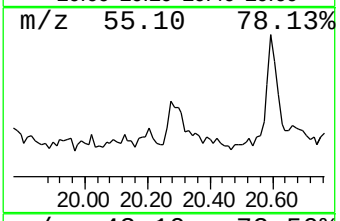
R.T.	EstConc	Area	Relative to ISTD	R.T.
20.27	2.56 ng	98861	Perylene-d12	18.80

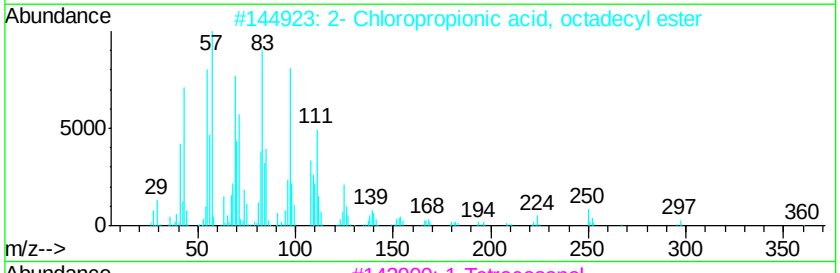
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	87
2	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	83
3	1-Tetracosanol	354	C24H50O	000506-51-4	80
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	76
5	Isotridecanol-	200	C13H28O	027458-92-0	72

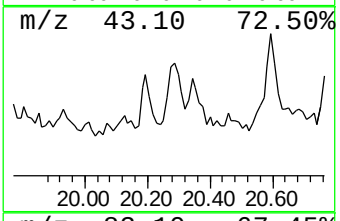


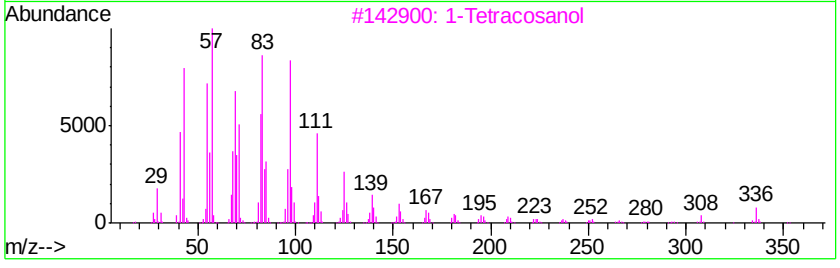


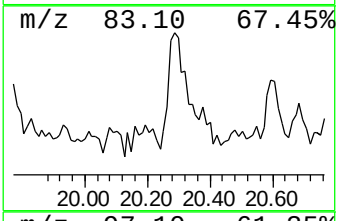


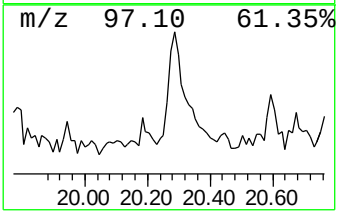












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ClientSampleId : SUP-B039(9-11)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

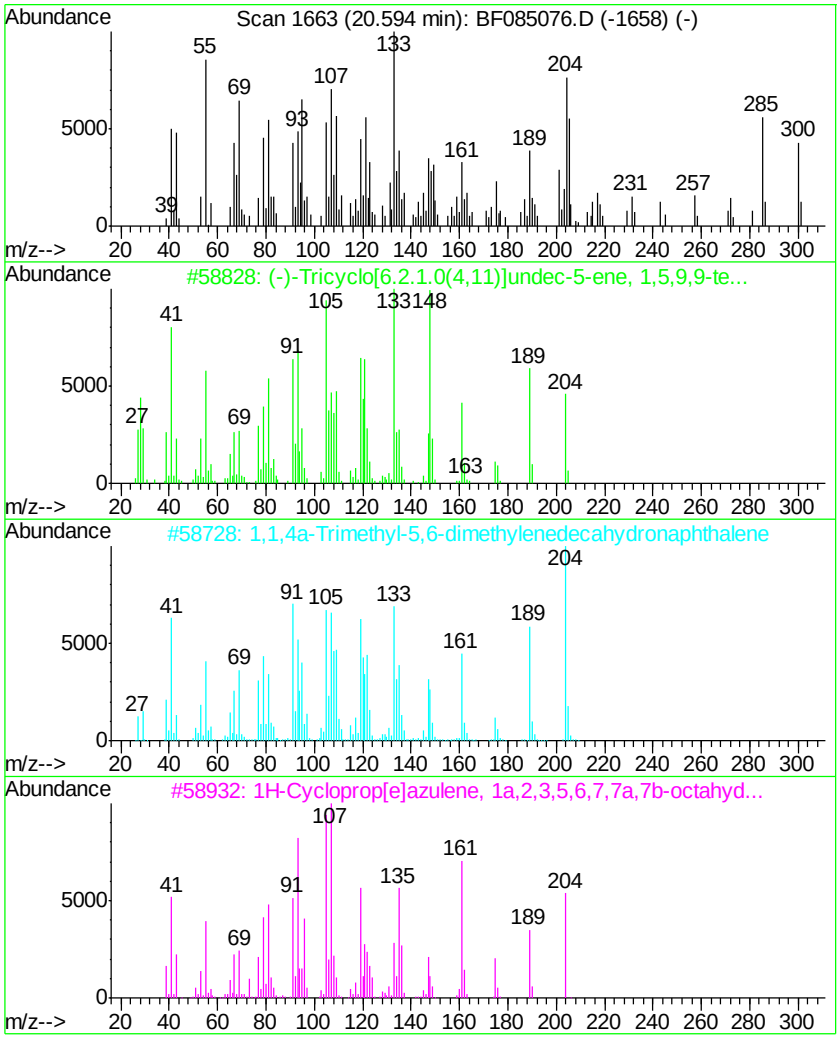
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

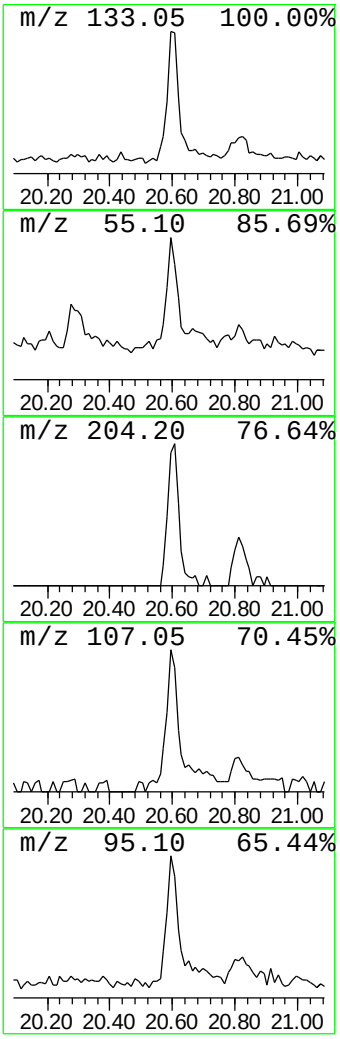
****

Peak Number 18 unknown20.59 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.59	10.36 ng	399575	Perylene-d12	18.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(-)-Tricyclo[6.2.1.0(4,11)]undec...	204	C15H24	1000154-06-7	49
2	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	46
3	1H-Cycloprop[e]azulene, 1a,2,3,5...	204	C15H24	021747-46-6	45
4	.beta.-Humulene	204	C15H24	000116-04-1	43
5	1,3-Benzodioxole, 5-(1-(4-ethoxy...	300	C18H20O4	090632-70-5	35





Tentatively Identified Compound (LSC) summary

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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
Butane, 2-methoxy...	1.68	3.2	ng	189909	1	5.91	1185290	20.0
2-Pentanone, 4-hy...	3.70	13.2	ng	783554	1	5.91	1185290	20.0
unknown5.56	5.56	109.1	ng	6465240	1	5.91	1185290	20.0
Eicosane	11.42	2.0	ng	140716	3	10.58	1387860	20.0
Heptacosane	14.93	15.7	ng	888933	4	13.01	1132730	20.0
Tritetracontane	17.11	22.1	ng	1004520	5	17.18	907195	20.0
17-Pentatriacontene	17.90	6.9	ng	311894	5	17.18	907195	20.0
Trifluoroacetic a...	18.58	10.3	ng	396536	6	18.80	771371	20.0
9-Tricosene, (Z)-	19.31	15.7	ng	604082	6	18.80	771371	20.0
unknown19.74	19.74	2.4	ng	92535	6	18.80	771371	20.0
2- Chloropropioni...	20.27	2.6	ng	98861	6	18.80	771371	20.0
unknown20.59	20.59	10.4	ng	399575	6	18.80	771371	20.0