LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050117\
Data File : BF094754.D
Acq On : 1 May 2017 16:33
Operator : SJ/MA
Sample : I2927-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-03-003-B

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-BF041717.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	3.931	335	339	352	rVB	319624	391963	15.26%	1.567%
2	4.325	403	406	422	rBV	2157971	2333921	90.84%	9.332%
3	4.642	457	460	467	rBV	159887	182064	7.09%	0.728%
4	5.401	584	589	602	rBV	2336908	2395987	93.25%	9.580%
5	5.519	605	609	615	rBV	2566983	2524057	98.24%	10.092%
6	5.760	647	650	654	rBV	647454	598302	23.29%	2.392%
7	5.942	676	681	684	rBV	2026683	1936022	75.35%	7.741%
8	6.413	756	761	764	rBV	1570479	1556349	60.57%	6.223%
9	6.589	787	791	798	rBV	32144	36714	1.43%	0.147%
10	7.254	900	904	907	rBV	891753	770998	30.01%	3.083%
11	7.278	907	908	916	rVB	72087	50913	1.98%	0.204%
12	8.578	1124	1129	1132	rBV	2764779	2569335	100.00%	10.273%
13	8.772	1157	1162	1165	rBV	30342	33715	1.31%	0.135%
14	9.083	1210	1215	1223	rBV	776566	739203	28.77%	2.956%
15	9.389	1260	1267	1271	rBV	852246	838963	32.65%	3.354%
16	9.425	1271	1273	1277	rVB	40712	39184	1.53%	0.157%
17	9.648	1308	1311	1316	rBV	24536	26629	1.04%	0.106%
18	9.983	1365	1368	1373	rVB	53633	45427	1.77%	0.182%
19	10.066	1378	1382	1387	rVB	46900	46615	1.81%	0.186%
20	10.260	1408	1415	1418	rBV4	21263	32861	1.28%	0.131%
21	10.366	1429	1433	1441	rBV	1136046	1254344	48.82%	5.015%
22	10.566	1463	1467	1470	rBV	60204	66419	2.59%	0.266%
23	11.124	1558	1562	1565	rVB	36768	36498	1.42%	0.146%
24	11.213	1573	1577	1580	rBV	710465	703901	27.40%	2.814%
25	11.242	1580	1582	1587	rVV	266495	232827	9.06%	0.931%
26	11.307	1587	1593	1597	rVV	70345	78829	3.07%	0.315%
27	11.519	1622	1629	1633	rBV2	25481	40543	1.58%	0.162%
28	11.560	1633	1636	1645	rVV	117683	172022	6.70%	0.688%
29	11.648	1648	1651	1659	rVB	30006	35054	1.36%	0.140%
30	11.836	1680	1683	1686	rBV	36613	41452	1.61%	0.166%
31	11.871	1686	1689	1692	rVB	44148	38718	1.51%	0.155%
32	11.948	1695	1702	1704	rBV3	86160	119374	4.65%	0.477%
33	11.966	1704	1705	1709	rVB	61498	45910	1.79%	0.184%
34	12.518	1795	1799	1802	rBV2	26619	33267	1.29%	0.133%

LSC Area Percent Report

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Data File : BF094754.D
Acq On : 1 May 2017 16:33
Operator : SJ/MA
Sample : I2927-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-03-003-B

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-BF041717.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.571	1802	1808	1815	rBV	388869	543670	21.16%	2.174%
36	12.707	1827	1831	1836	rBV	309585	339121	13.20%	1.356%
37	12.918	1863	1867	1869	rBV3	24633	29917	1.16%	0.120%
38	12.977	1873	1877	1881	rVB	299890	329805	12.84%	1.319%
39	13.189	1909	1913	1917	rBV	1605961	1689694	65.76%	6.756%
40	13.395	1946	1948	1956	rVB	54572	66347	2.58%	0.265%
41	13.477	1960	1962	1965	rBV	31053	29975	1.17%	0.120%
42	13.524	1967	1970	1975	rVV4	31284	48680	1.89%	0.195%
43	13.783	2010	2014	2019	rVB	96681	126222	4.91%	0.505%
44	14.360	2108	2112	2119	rBV3	74805	131557	5.12%	0.526%
45	14.465	2125	2130	2133	rBV2	570241	700064	27.25%	2.799%
46	14.495	2133	2135	2137	rVV	73083	63774	2.48%	0.255%
47	15.695	2336	2339	2342	rBV	112356	160269	6.24%	0.641%
48	15.983	2386	2388	2394	rVB	81523	88012	3.43%	0.352%
49	16.042	2395	2398	2403	rVB	104487	127060	4.95%	0.508%
50	16.095	2403	2407	2411	rBV	453657	487996	18.99%	1.951%

Sum of corrected areas: 25010543

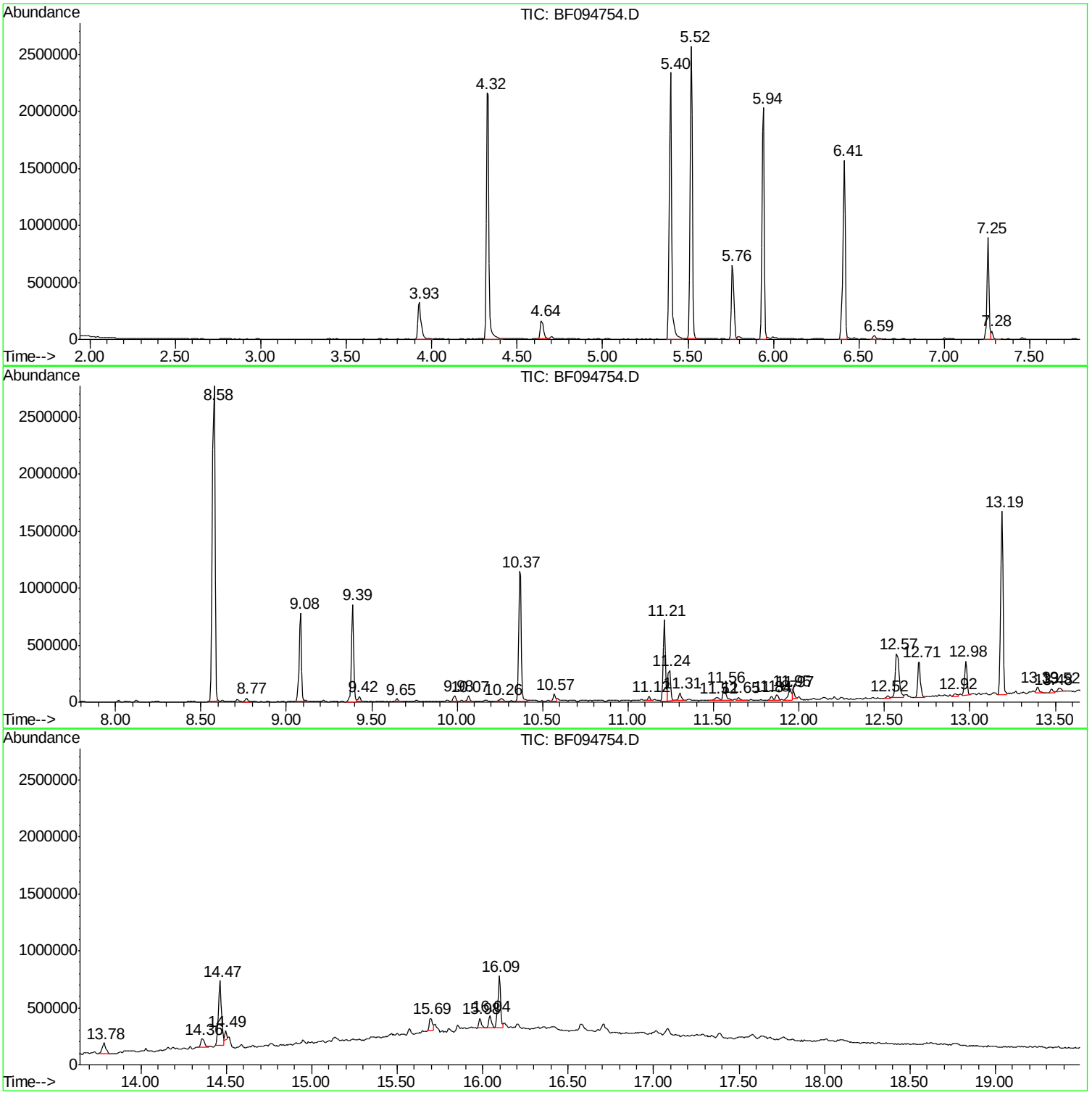
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050117\
Data File : BF094754.D
Acq On : 1 May 2017 16:33
Operator : SJ/MA
Sample : I2927-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-03-003-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF050117\
Data File : BF094754.D
Acq On : 1 May 2017 16:33
Operator : SJ/MA
Sample : I2927-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-03-003-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

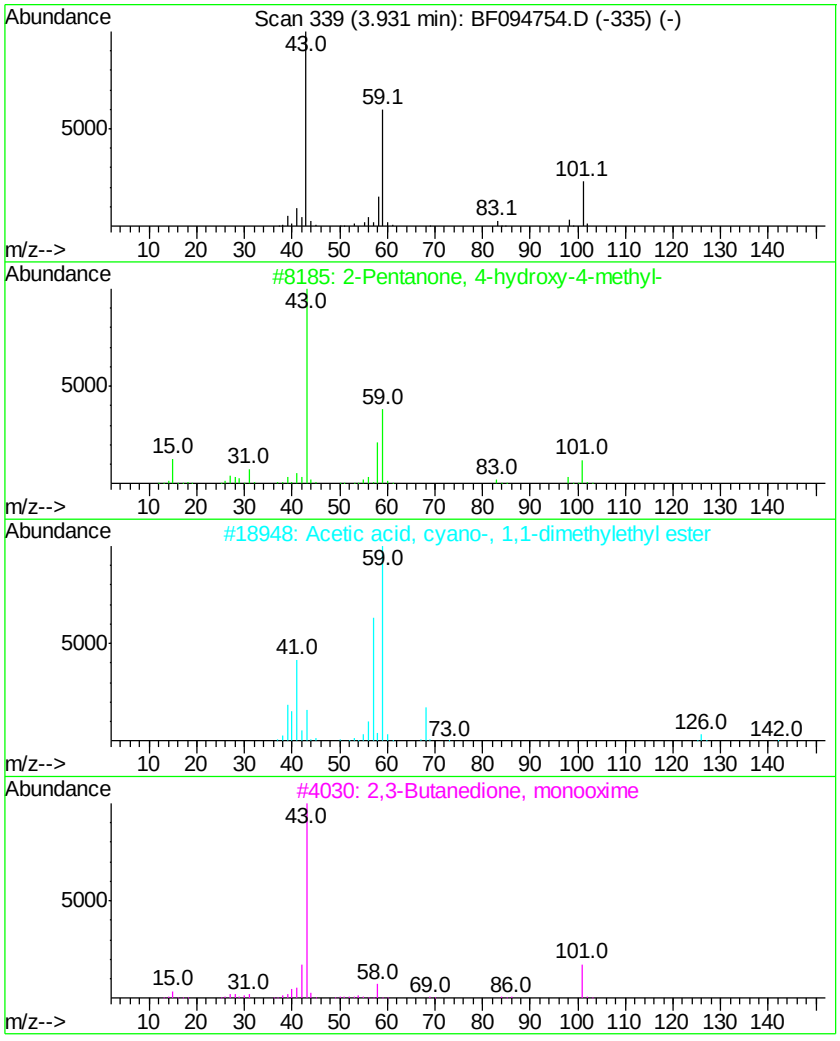
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

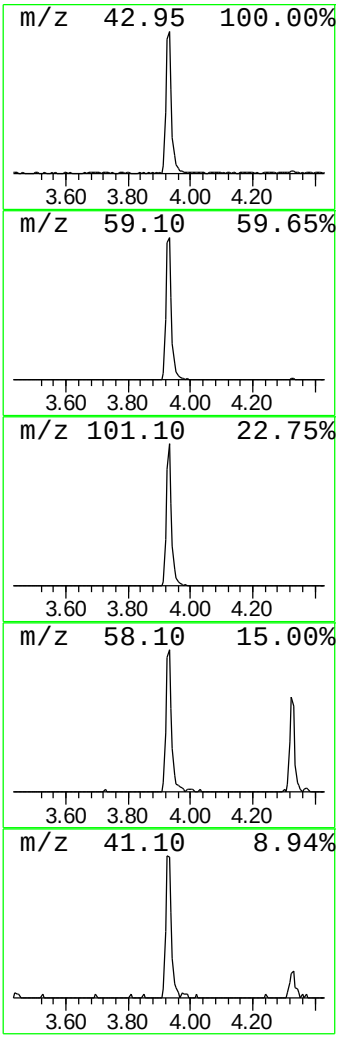
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.93	13.10 ng	391963	1,4-Dichlorobenzene-d4	5.76

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	17
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050117\
Data File : BF094754.D
Acq On : 1 May 2017 16:33
Operator : SJ/MA
Sample : I2927-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-03-003-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

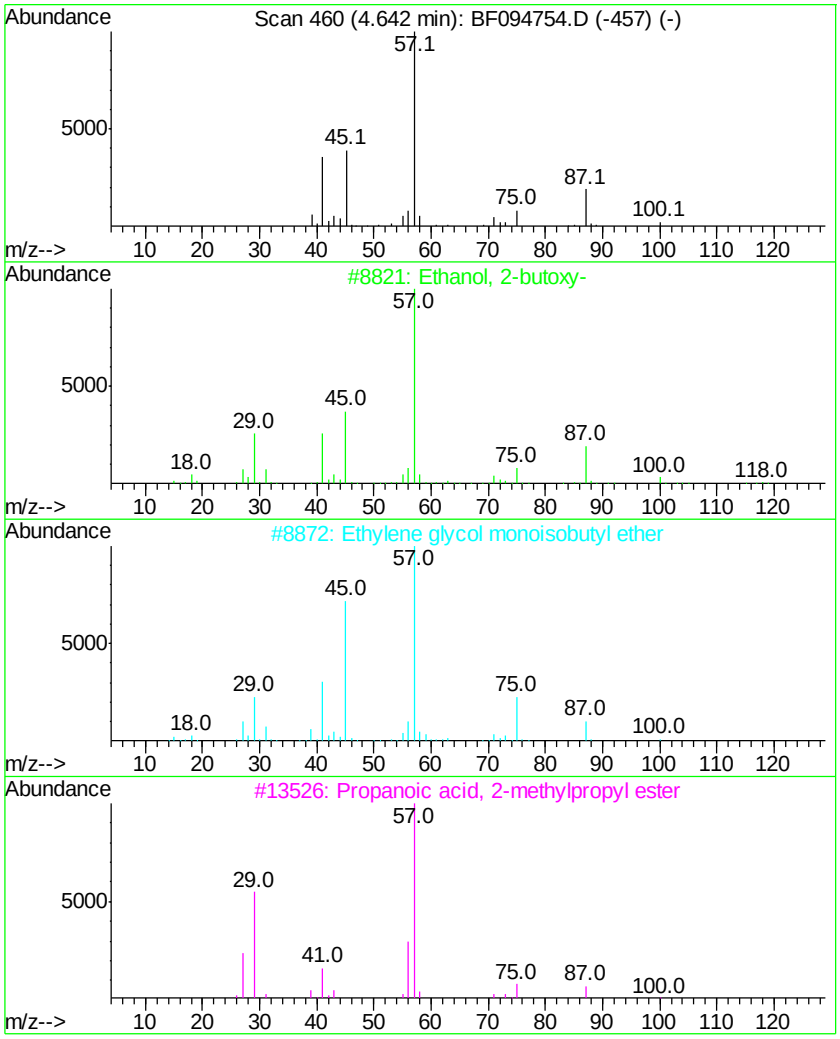
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

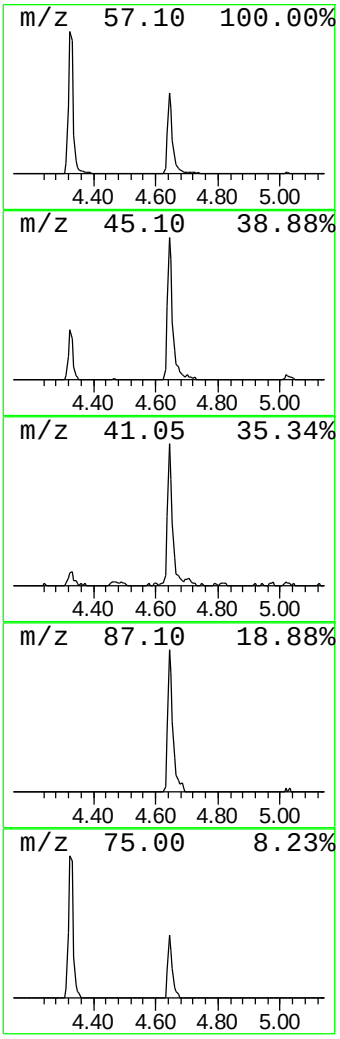
****

Peak Number 2 Ethanol, 2-butoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.64	6.09 ng	182064	1,4-Dichlorobenzene-d4	5.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	74
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	53
3	Propanoic acid, 2-methylpropyl e...	130	C7H14O2	000540-42-1	16
4	n-Butyl ether	130	C8H18O	000142-96-1	16
5	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	12





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050117\
Data File : BF094754.D
Acq On : 1 May 2017 16:33
Operator : SJ/MA
Sample : I2927-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-03-003-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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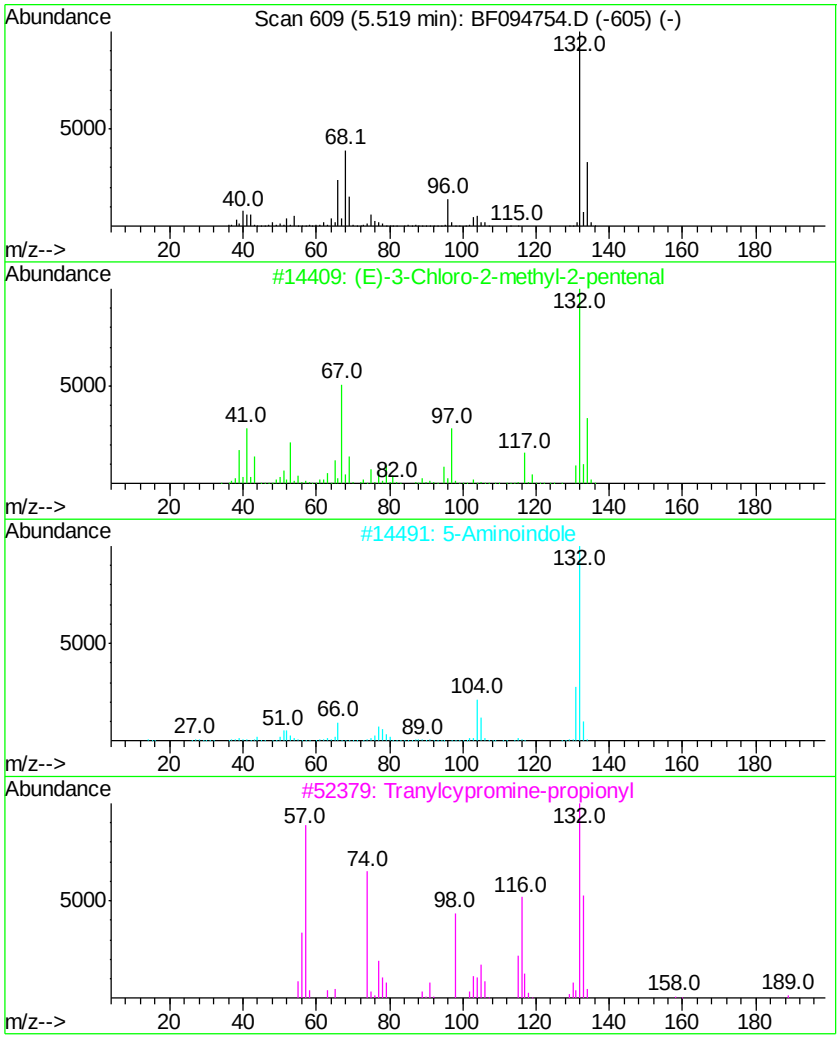
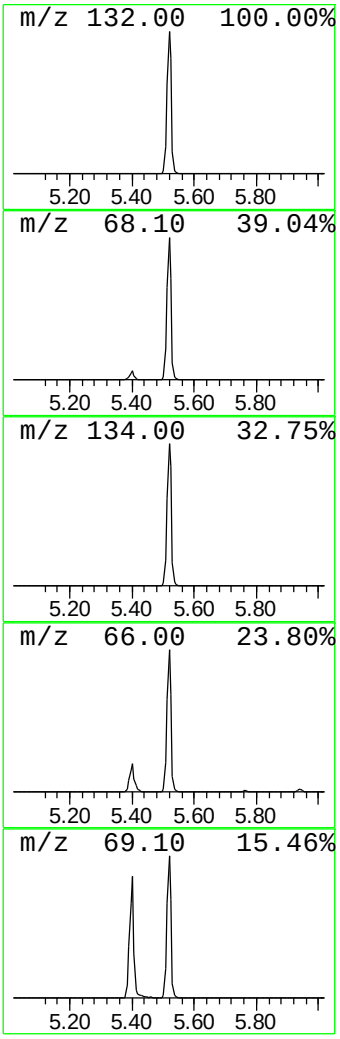
Peak Number 3 unknown5.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.52	84.37 ng	2524060	1,4-Dichlorobenzene-d4	5.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050117\
Data File : BF094754.D
Acq On : 1 May 2017 16:33
Operator : SJ/MA
Sample : I2927-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-03-003-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

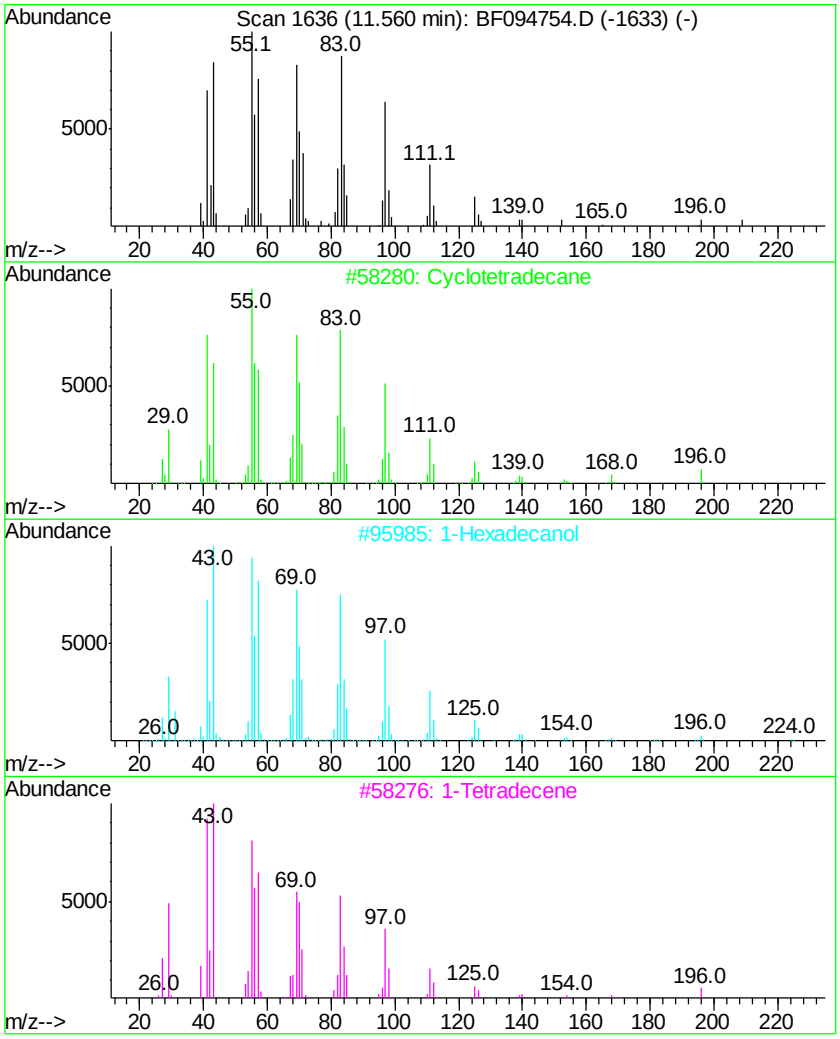
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

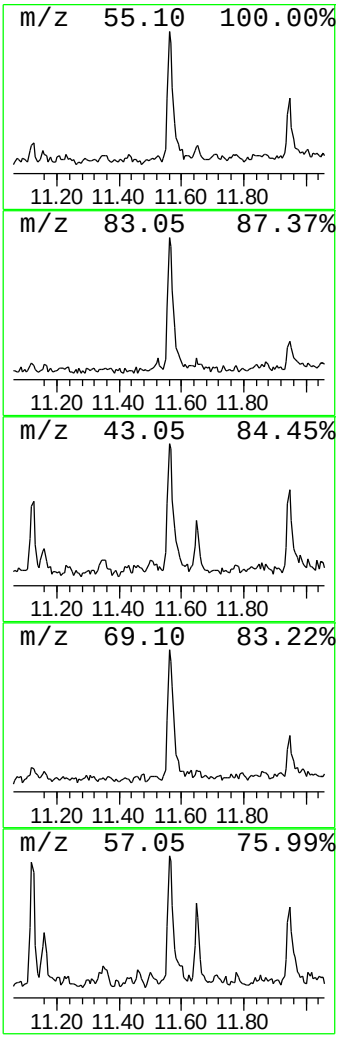
****

Peak Number 6 Cyclotetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.56	4.89 ng	172022	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	96
2	1-Hexadecanol	242	C16H34O	036653-82-4	95
3	1-Tetradecene	196	C14H28	001120-36-1	91
4	2-Tetradecene, (E)-	196	C14H28	035953-54-9	91
5	n-Tridecan-1-ol	200	C13H28O	000112-70-9	91





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050117\
Data File : BF094754.D
Acq On : 1 May 2017 16:33
Operator : SJ/MA
Sample : I2927-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-03-003-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

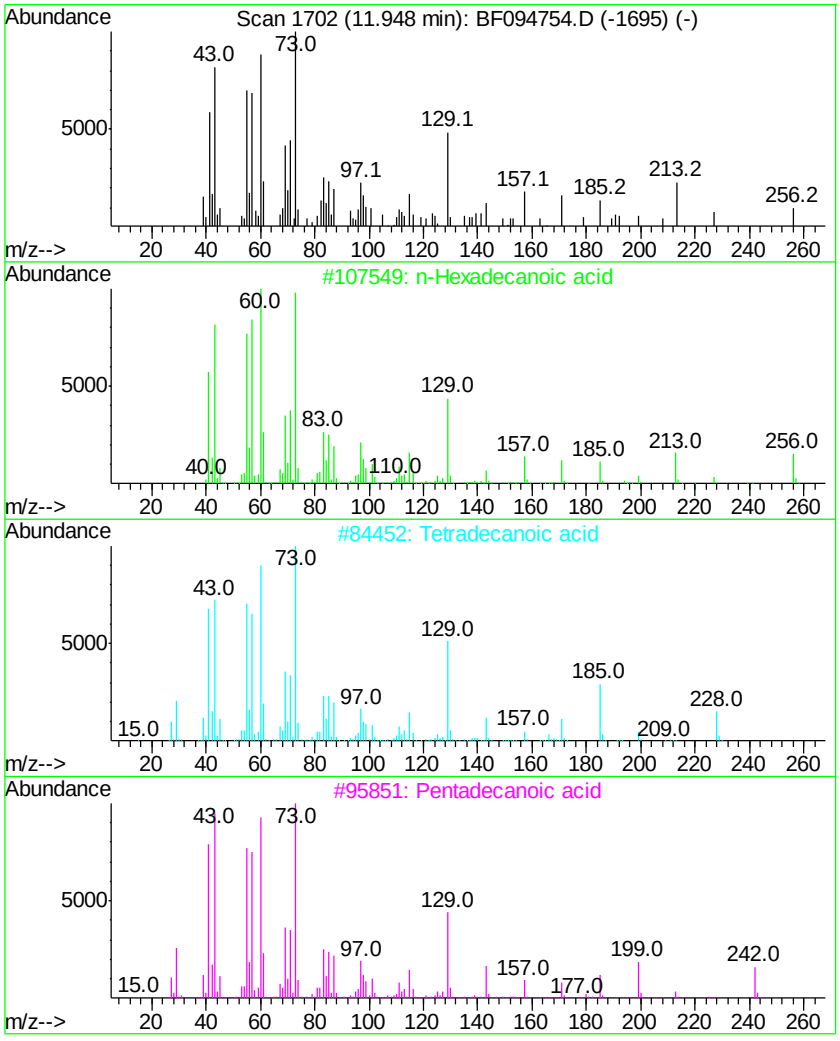
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

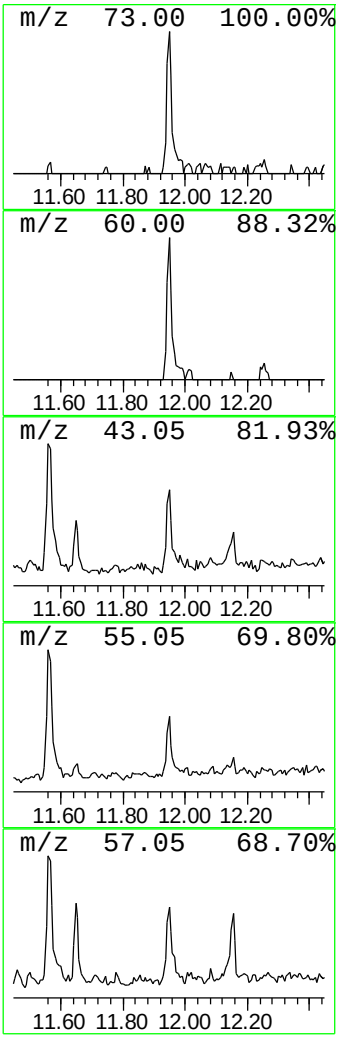
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	3.39 ng	119374	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050117\
Data File : BF094754.D
Acq On : 1 May 2017 16:33
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Sample : I2927-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-03-003-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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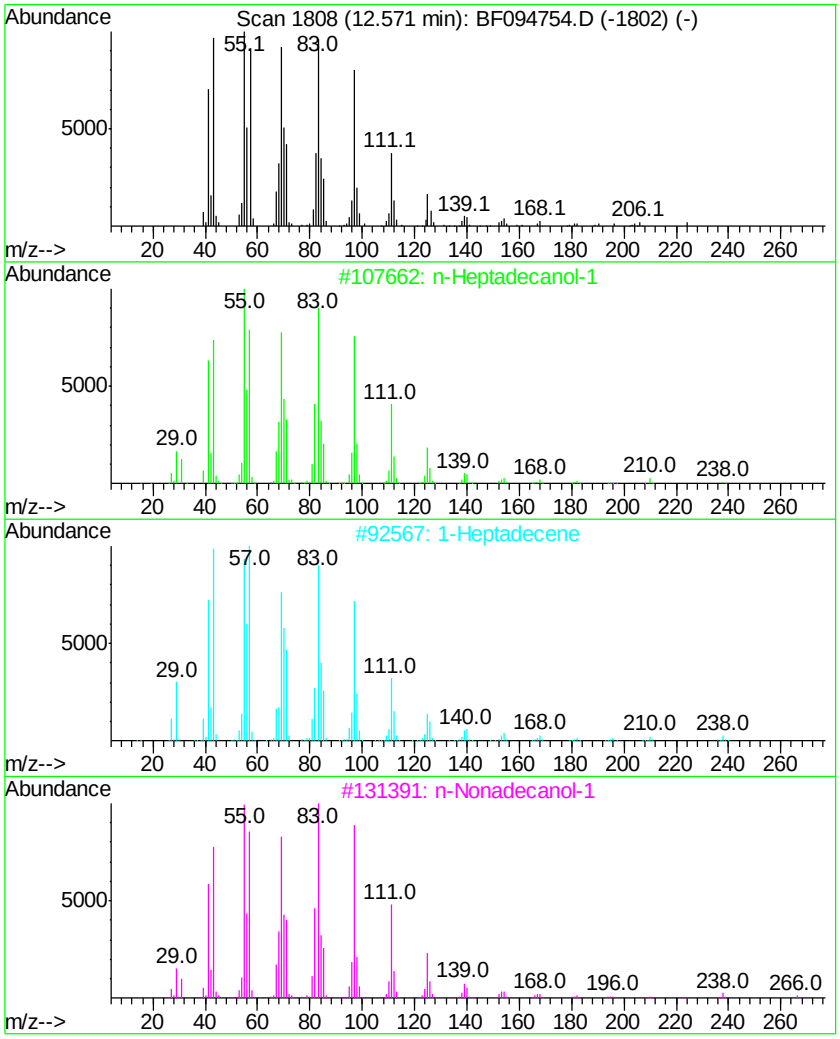
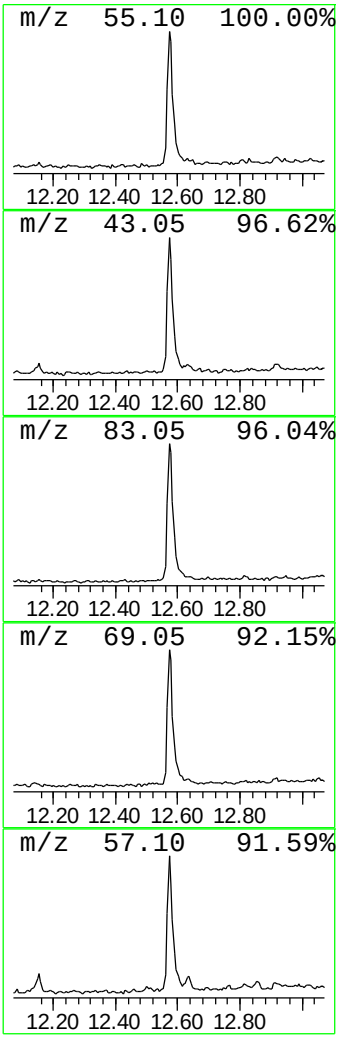
Peak Number 8 n-Heptadecanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	15.45 ng	543670	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Heptadecanol-1	256	C17H36O	001454-85-9	95
2	1-Heptadecene	238	C17H34	006765-39-5	94
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	94
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94





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Sample : I2927-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-03-003-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

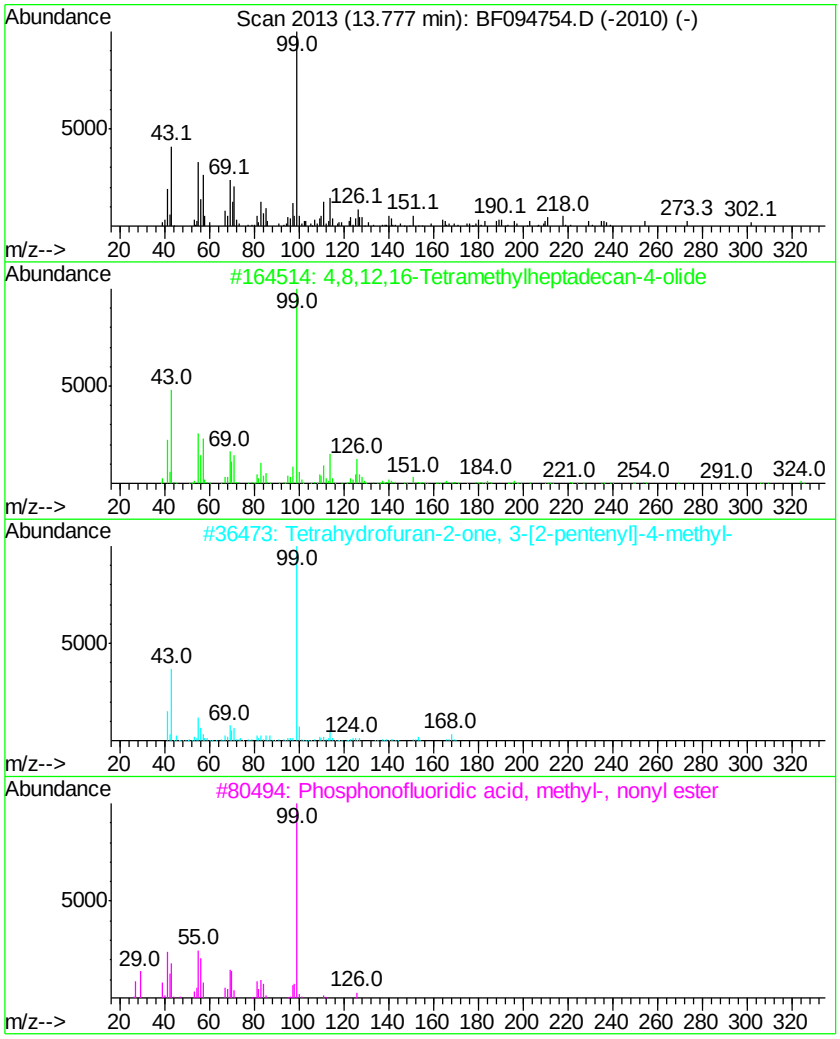
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

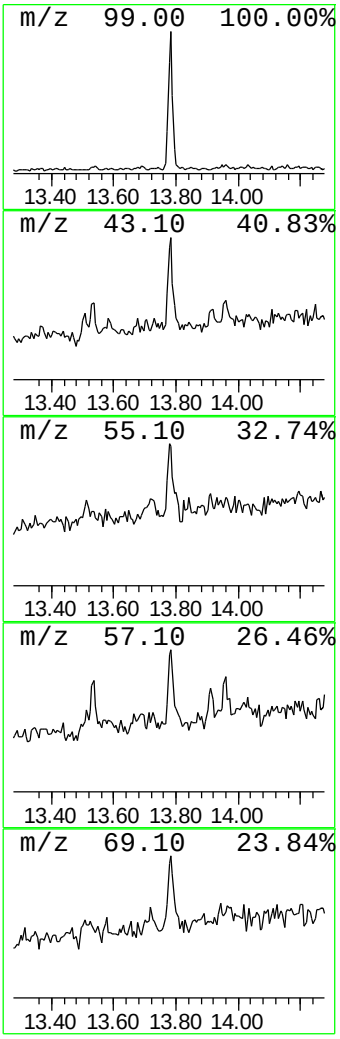
****

Peak Number 9 4,8,12,16-Tetramethylheptad... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.78	3.61 ng	126222	Chrysene-d12	14.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,8,12,16-Tetramethylheptadecan-...	324	C21H40O2	096168-15-9	87
2	Tetrahydrofuran-2-one, 3-[2-pent...	168	C10H16O2	1000132-08-6	59
3	Phosphonofluoridic acid, methyl-...	224	C10H22FO2P	211192-74-4	50
4	Hexanoic acid, 4-hexadecyl ester	340	C22H44O2	1000282-83-8	50
5	Hexanoic acid, but-3-yn-2-yl ester	168	C10H16O2	1000299-35-1	50





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050117\
Data File : BF094754.D
Acq On : 1 May 2017 16:33
Operator : SJ/MA
Sample : I2927-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-03-003-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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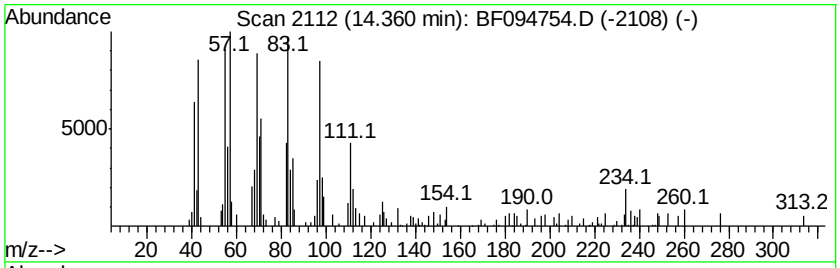
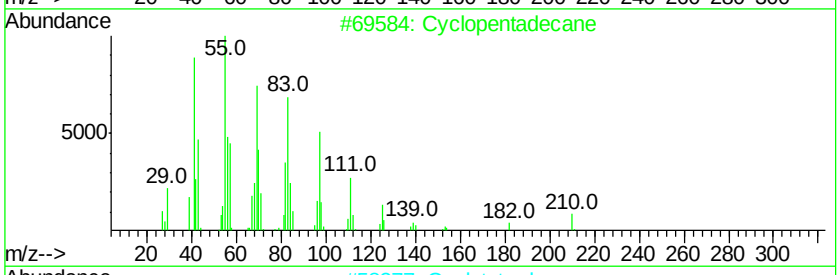
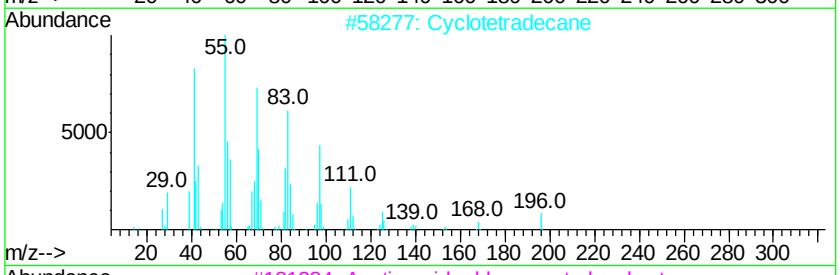
Peak Number 10 Cyclopentadecane Concentration Rank 7

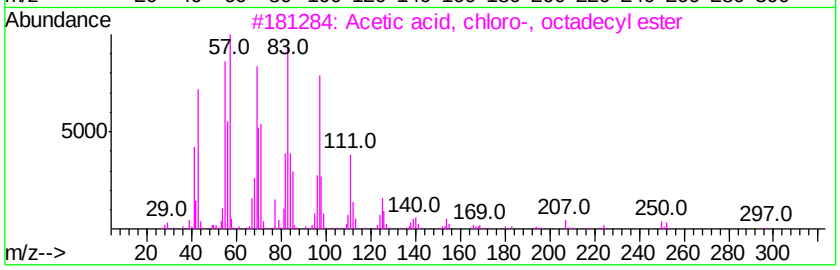
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	3.76 ng	131557	Chrysene-d12	14.47

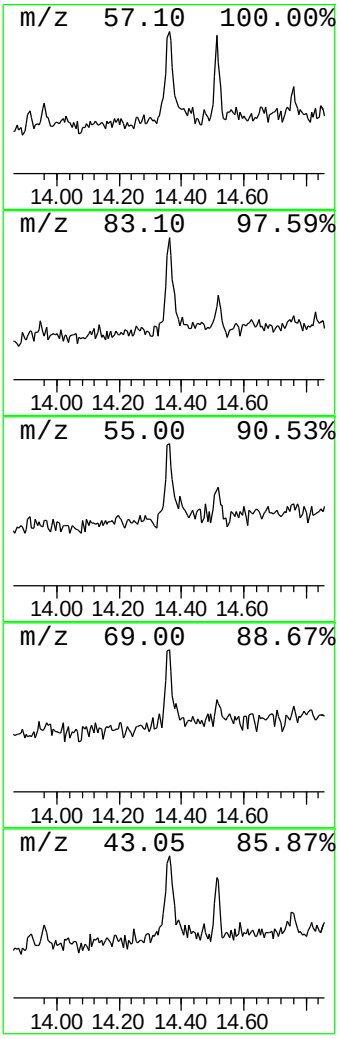
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	93
2	Cyclotetradecane	196	C14H28	000295-17-0	93
3	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	93
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93











Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050117\
Data File : BF094754.D
Acq On : 1 May 2017 16:33
Operator : SJ/MA
Sample : I2927-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-03-003-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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...	3.93	13.1	ng	391963	1	5.76	598302	20.0
Ethanol, 2-butoxy-	4.64	6.1	ng	182064	1	5.76	598302	20.0
unknown5.52	5.52	84.4	ng	2524060	1	5.76	598302	20.0
Cyclotetradecane	11.56	4.9	ng	172022	4	11.21	703901	20.0
n-Hexadecanoic acid	11.95	3.4	ng	119374	4	11.21	703901	20.0
n-Heptadecanol-1	12.57	15.4	ng	543670	4	11.21	703901	20.0
4,8,12,16-Tetrame...	13.78	3.6	ng	126222	5	14.47	700064	20.0
Cyclopentadecane	14.36	3.8	ng	131557	5	14.47	700064	20.0