LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102731.D
Acq On : 5 Feb 2018 11:58
Operator : SJ/JU
Sample : J1436-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B15

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-BF020318.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	2.169	9	14	19	rVB	453126	577094	10.39%	1.186%
2	5.122	512	516	522	rVB	146517	201041	3.62%	0.413%
3	5.498	574	580	583	rBV	4997790	5457550	98.22%	11.213%
4	6.510	745	752	764	rVB	4688790	5556486	100.00%	11.416%
5	6.651	771	776	779	rBV	5252216	5371025	96.66%	11.035%
6	6.881	811	815	819	rBV	1707802	1365791	24.58%	2.806%
7	7.039	837	842	845	rVB	4484446	4037600	72.66%	8.295%
8	7.445	905	911	914	rBV	3543813	3518585	63.32%	7.229%
9	8.163	1029	1033	1036	rBV	2277278	1811632	32.60%	3.722%
10	9.239	1211	1216	1219	rBV	5671509	5341802	96.14%	10.975%
11	9.627	1278	1282	1285	rBV	605603	454646	8.18%	0.934%
12	9.845	1317	1319	1322	rVB	91820	66358	1.19%	0.136%
13	9.916	1327	1331	1335	rVB	1990700	1895568	34.11%	3.895%
14	10.345	1402	1404	1407	rVB	99885	72365	1.30%	0.149%
15	10.633	1448	1453	1459	rBV	106011	108809	1.96%	0.224%
16	10.710	1459	1466	1469	rBV	3154147	3185675	57.33%	6.545%
17	10.816	1481	1484	1490	rVB	83067	96320	1.73%	0.198%
18	11.263	1557	1560	1563	rBV	64266	60544	1.09%	0.124%
19	11.404	1580	1584	1588	rBV	1948584	1689445	30.40%	3.471%
20	11.927	1669	1673	1678	rBV	739426	727344	13.09%	1.494%
21	12.710	1802	1806	1814	rBV	496751	531071	9.56%	1.091%
22	12.804	1819	1822	1825	rVB	109164	98042	1.76%	0.201%
23	12.880	1833	1835	1839	rVB	118537	97227	1.75%	0.200%
24	12.992	1849	1854	1857	rBV	3881915	3846113	69.22%	7.902%
25	13.462	1932	1934	1939	rVB	86684	80588	1.45%	0.166%
26	13.874	2001	2004	2016	rVB	319415	329833	5.94%	0.678%
27	14.039	2029	2032	2036	rVB	1057845	1027375	18.49%	2.111%
28	15.521	2279	2284	2293	rBV	830350	1066305	19.19%	2.191%

Sum of corrected areas: 48672234

LSC Report - Integrated Chromatogram

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Misc :
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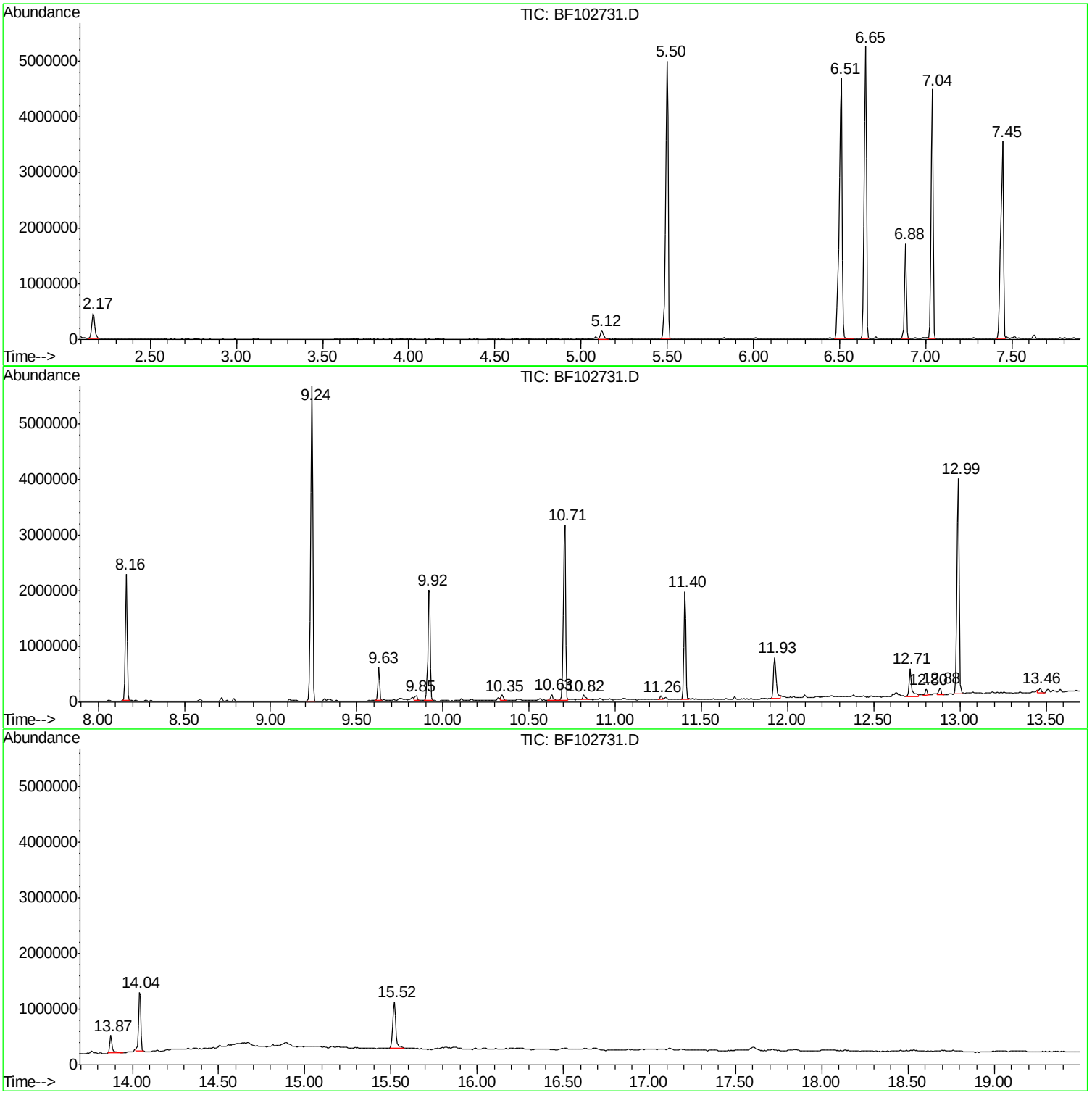
Instrument : BNA_F
ClientSampleId : B15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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Acq On : 5 Feb 2018 11:58
Operator : SJ/JU
Sample : J1436-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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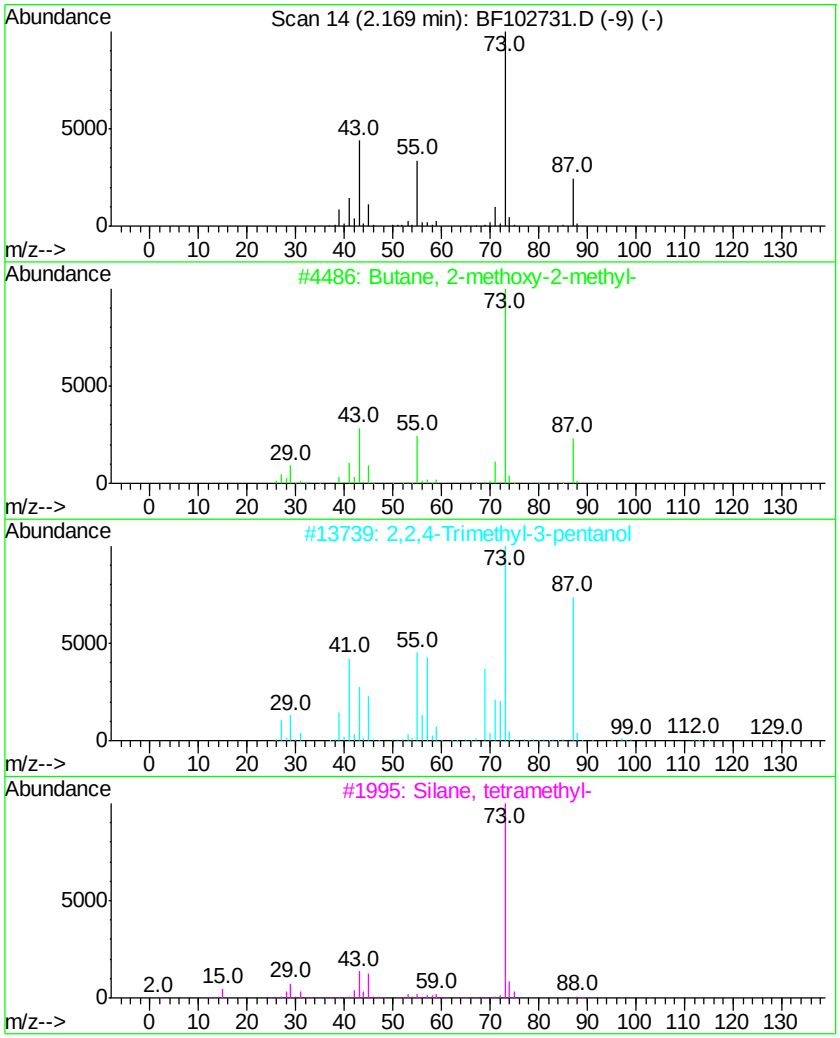
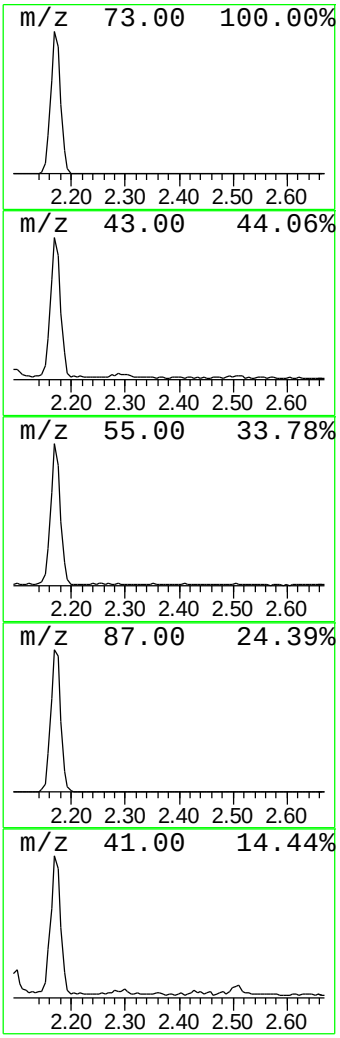
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	8.45 ng	577094	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Sample : J1436-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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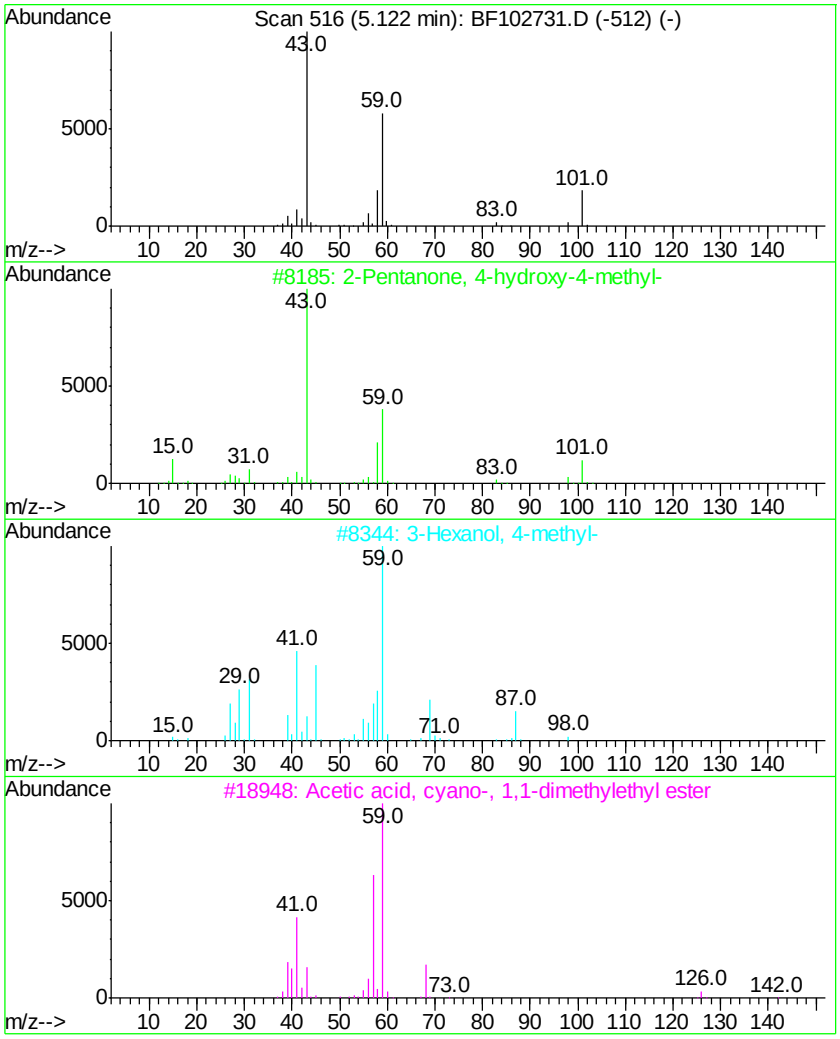
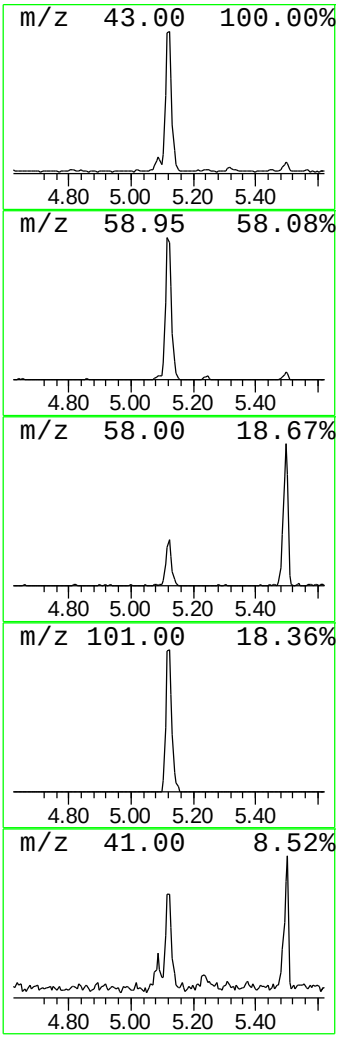
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	2.94 ng	201041	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5	Acetone	58	C3H6O	000067-64-1	9





Library Search Compound Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102731.D
Acq On : 5 Feb 2018 11:58
Operator : SJ/JU
Sample : J1436-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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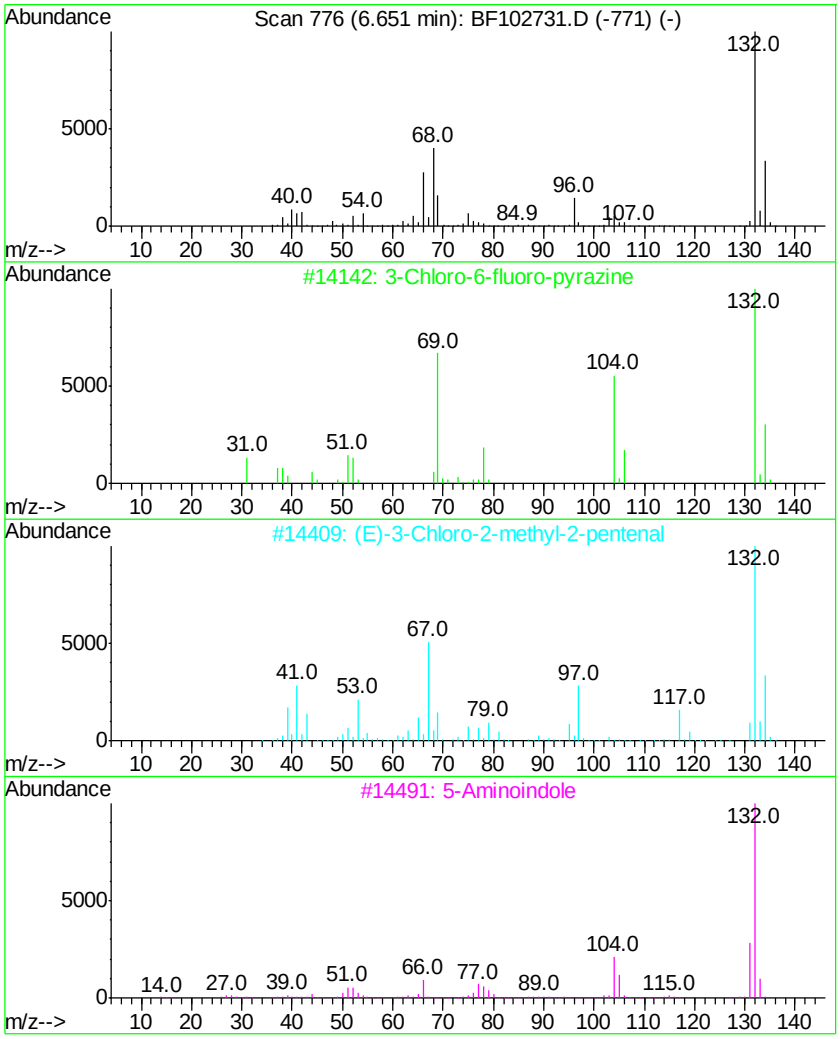
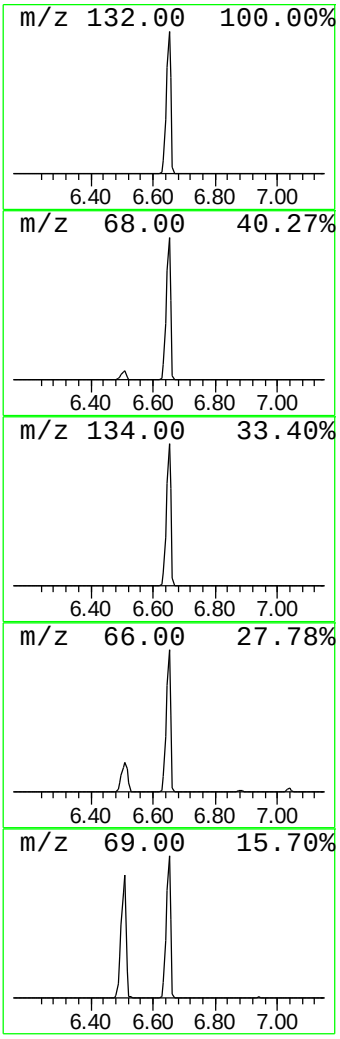
Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	78.65 ng	5371030	1,4-Dichlorobenzene-d4	6.88

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	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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ClientSampleId : B15

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TIC Library : C:\DATABASE\NIST11.L
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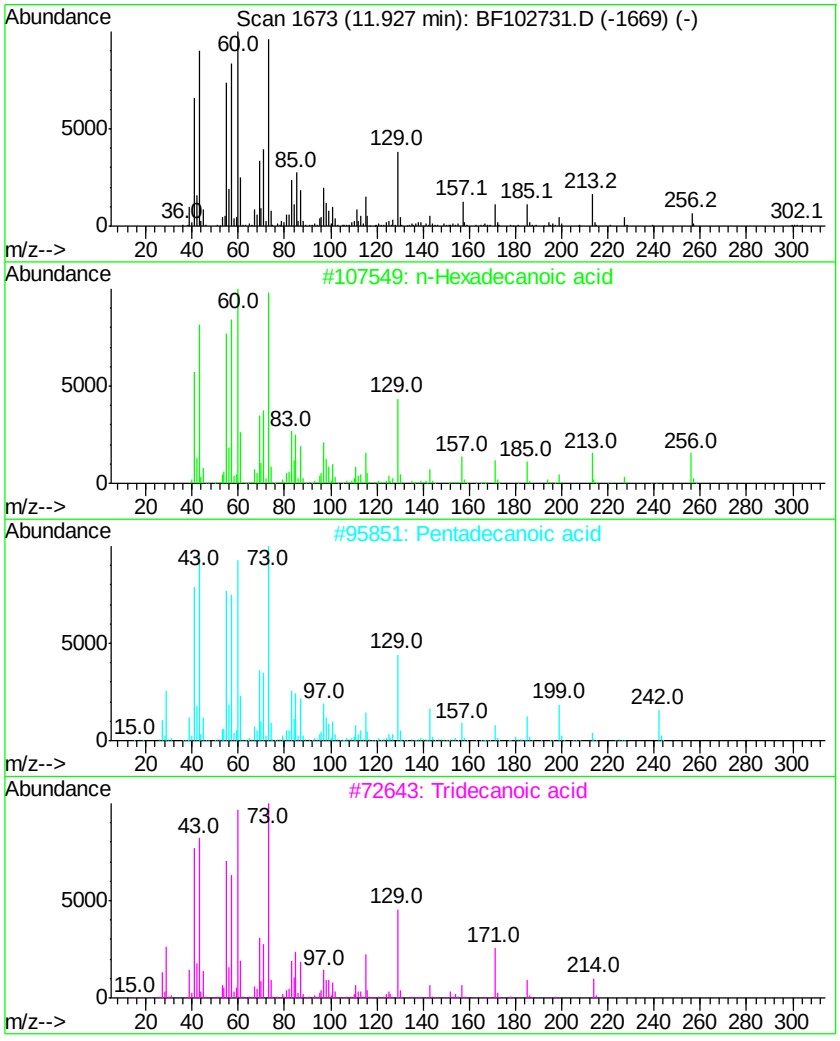
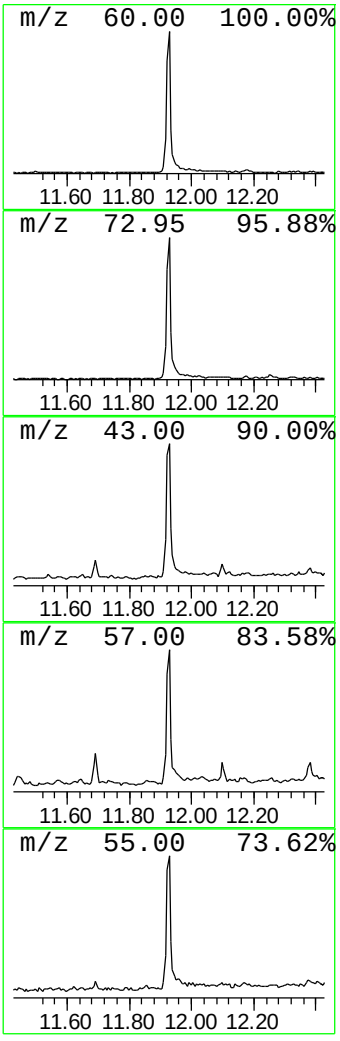
Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	8.61 ng	727344	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Octadecanoic acid	284	C18H36O2	000057-11-4	90
5	Dodecanoic acid	200	C12H24O2	000143-07-7	80





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Sample : J1436-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
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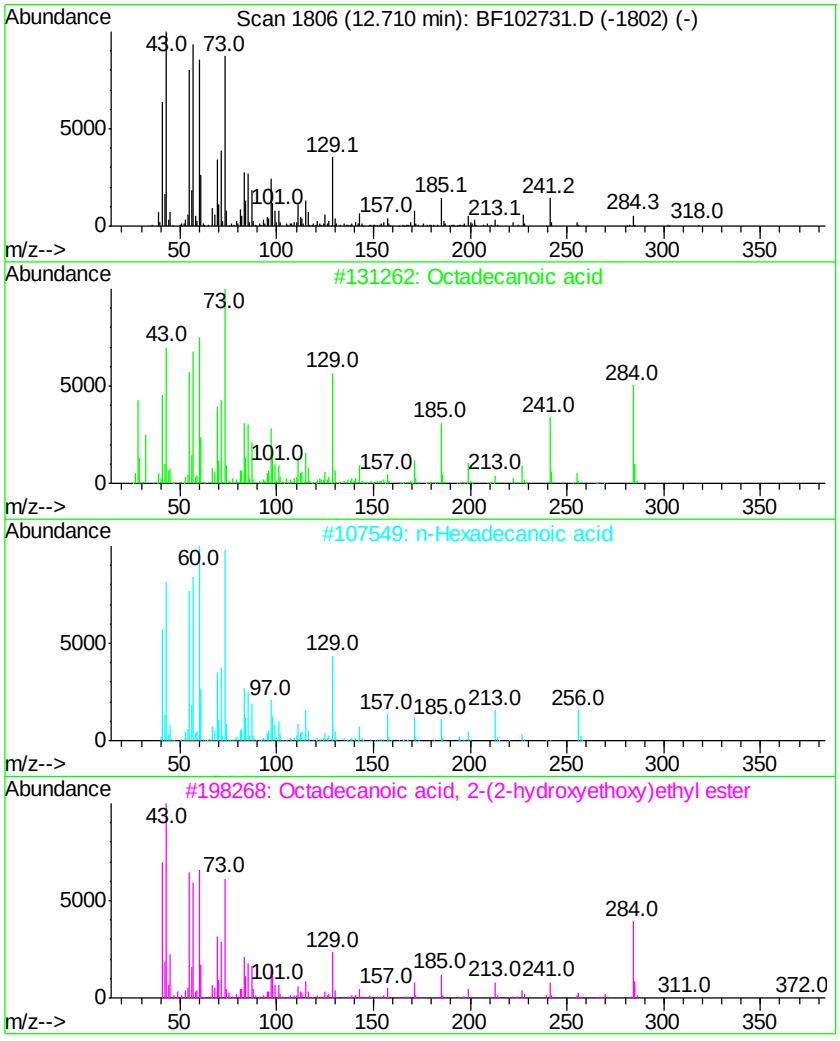
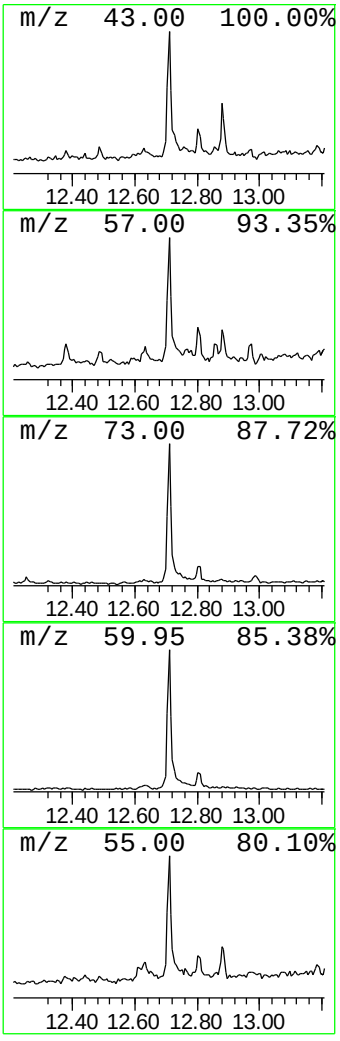
Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	6.29 ng	531071	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	86





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Instrument : BNA_F
ClientSampleId : B15

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

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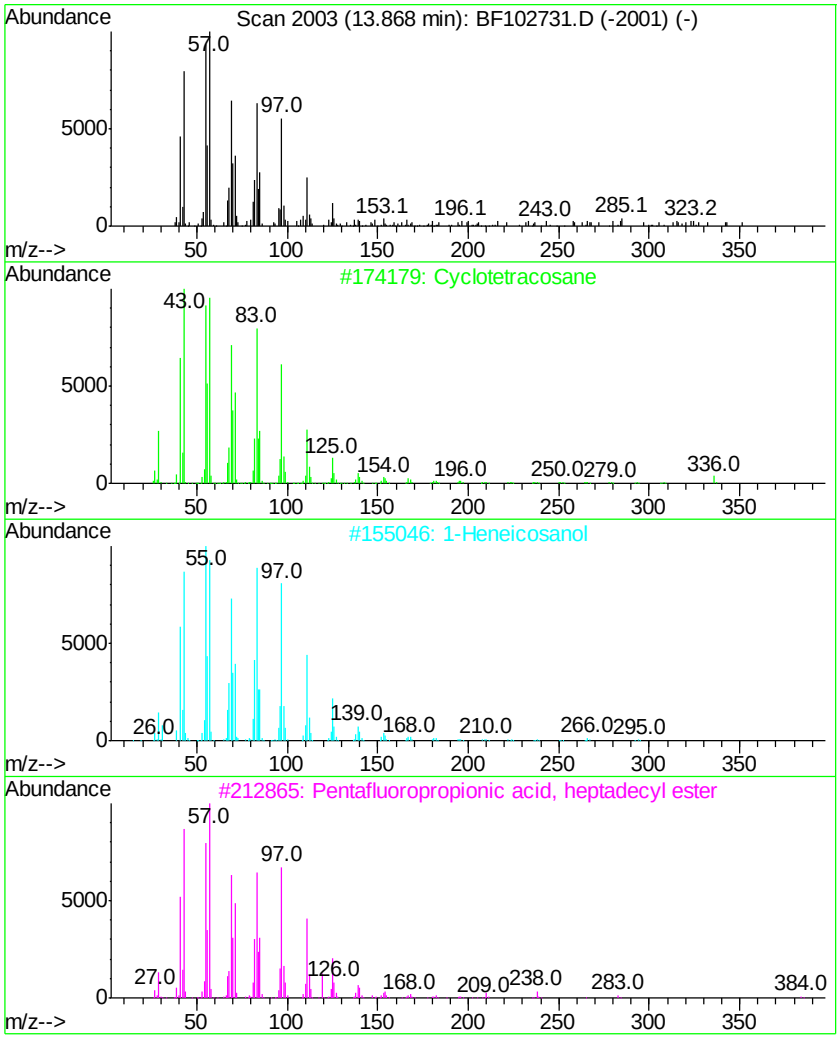
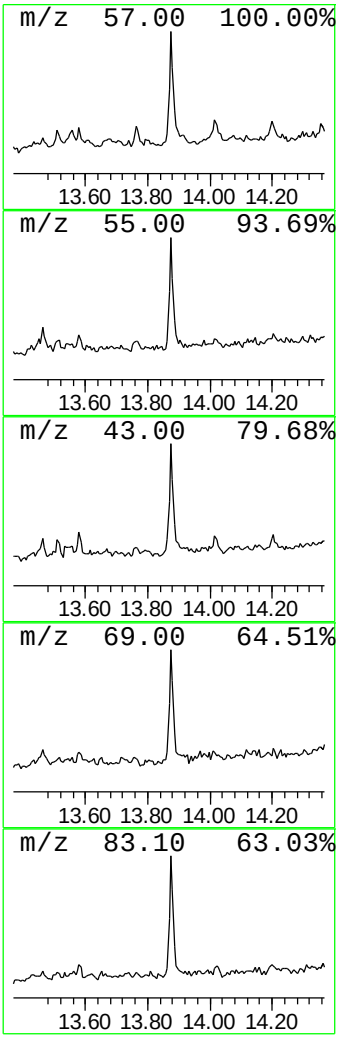
Peak Number 7 Cyclotetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	6.42 ng	329833	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	94
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5	Octacosanol	410	C28H58O	000557-61-9	91





Tentatively Identified Compound (LSC) summary

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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
Butane, 2-methoxy...	2.17	8.4	ng	577094	1	6.88	1365790	20.0
2-Pentanone, 4-hy...	5.12	2.9	ng	201041	1	6.88	1365790	20.0
unknown6.65	6.65	78.7	ng	5371030	1	6.88	1365790	20.0
n-Hexadecanoic acid	11.93	8.6	ng	727344	4	11.40	1689450	20.0
Octadecanoic acid	12.71	6.3	ng	531071	4	11.40	1689450	20.0
Cyclotetracosane	13.87	6.4	ng	329833	5	14.04	1027380	20.0