LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF020318\
Data File : BF102723.D
Acq On : 3 Feb 2018 18:03
Operator : SJ/JU
Sample : J1436-17
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B25

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	2.163	7	13	20	rVB	424918	546114	11.29%	1.292%
2	5.110	511	514	524	rVB	228431	290160	6.00%	0.686%
3	5.498	574	580	583	rBV	4528056	4800379	99.22%	11.354%
4	6.504	745	751	755	rBV	4257733	4838251	100.00%	11.444%
5	6.651	770	776	779	rBV	4405766	4719694	97.55%	11.163%
6	6.881	811	815	818	rBV	1425290	1190342	24.60%	2.815%
7	7.033	837	841	845	rVB	3610385	3518188	72.72%	8.321%
8	7.439	905	910	913	rBV	2984046	2983802	61.67%	7.057%
9	8.163	1028	1033	1036	rBV	1850711	1599841	33.07%	3.784%
10	8.710	1123	1126	1130	rBV	100767	84354	1.74%	0.200%
11	9.239	1211	1216	1219	rBV	4868041	4653243	96.18%	11.006%
12	9.627	1278	1282	1285	rBV	474157	383515	7.93%	0.907%
13	9.839	1316	1318	1323	rVB	72718	60077	1.24%	0.142%
14	9.916	1327	1331	1335	rVB2	1976698	1647557	34.05%	3.897%
15	10.216	1377	1382	1385	rBV	66110	81142	1.68%	0.192%
16	10.339	1401	1403	1407	rVB	88812	75476	1.56%	0.179%
17	10.627	1447	1452	1459	rVB	255441	221075	4.57%	0.523%
18	10.704	1459	1465	1468	rBV	2826290	2579656	53.32%	6.102%
19	10.804	1479	1482	1489	rVB2	74682	117295	2.42%	0.277%
20	11.263	1558	1560	1564	rBV2	47881	48647	1.01%	0.115%
21	11.404	1580	1584	1587	rBV	1461983	1337197	27.64%	3.163%
22	11.921	1665	1672	1689	rBV	545502	689182	14.24%	1.630%
23	12.627	1787	1792	1797	rBV7	40477	73834	1.53%	0.175%
24	12.704	1802	1805	1810	rBV	268561	303938	6.28%	0.719%
25	12.986	1849	1853	1856	rBV	3374785	3032035	62.67%	7.172%
26	13.874	2001	2004	2007	rBV	356755	326542	6.75%	0.772%
27	13.904	2007	2009	2014	rVB	95015	86153	1.78%	0.204%
28	14.039	2028	2032	2035	rBV	1094352	970865	20.07%	2.296%
29	15.515	2278	2283	2287	rBV	775156	1020126	21.08%	2.413%

Sum of corrected areas: 42278680

LSC Report - Integrated Chromatogram

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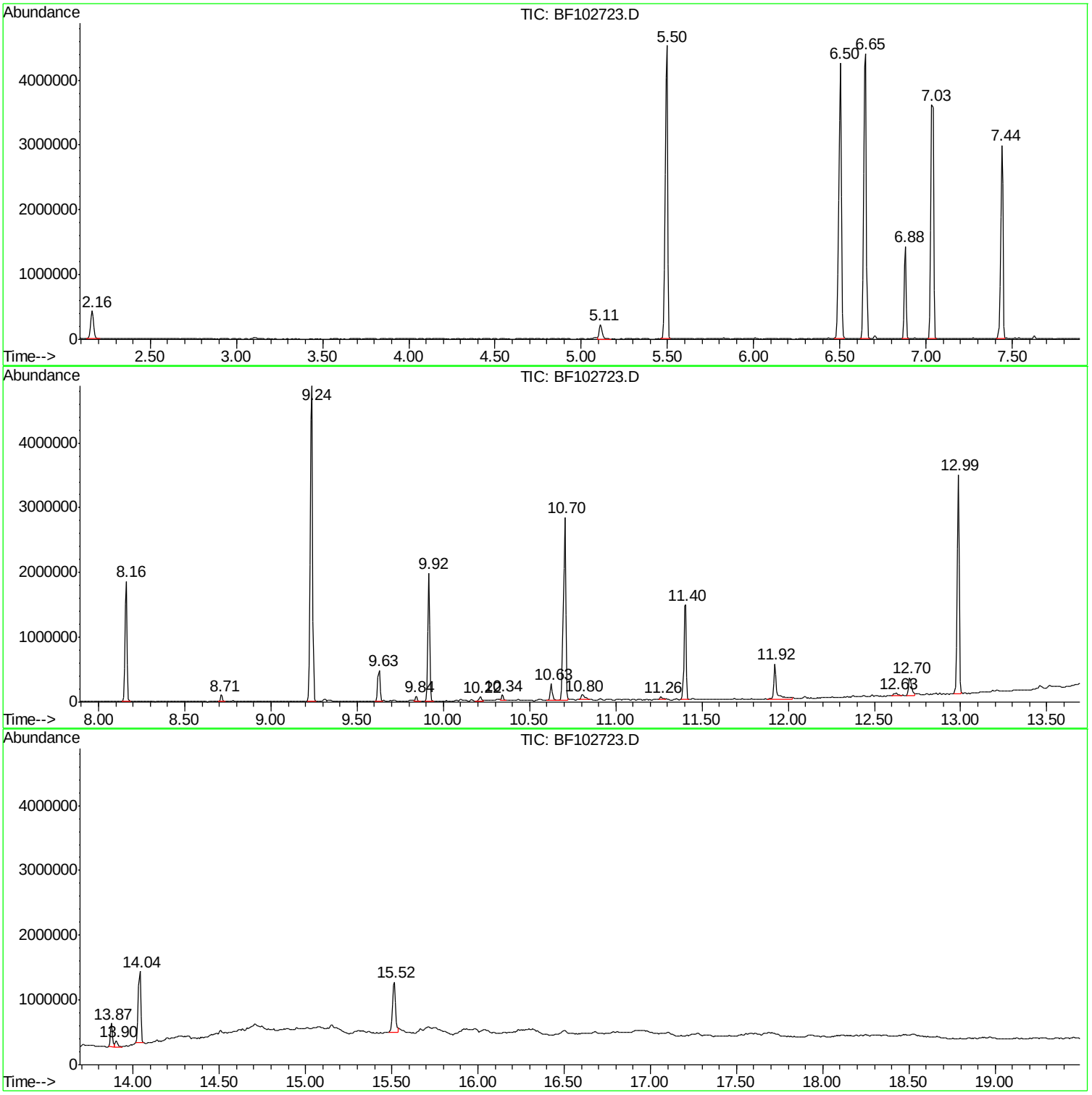
Acq On : 3 Feb 2018 18:03
Operator : SJ/JU
Sample : J1436-17
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B25

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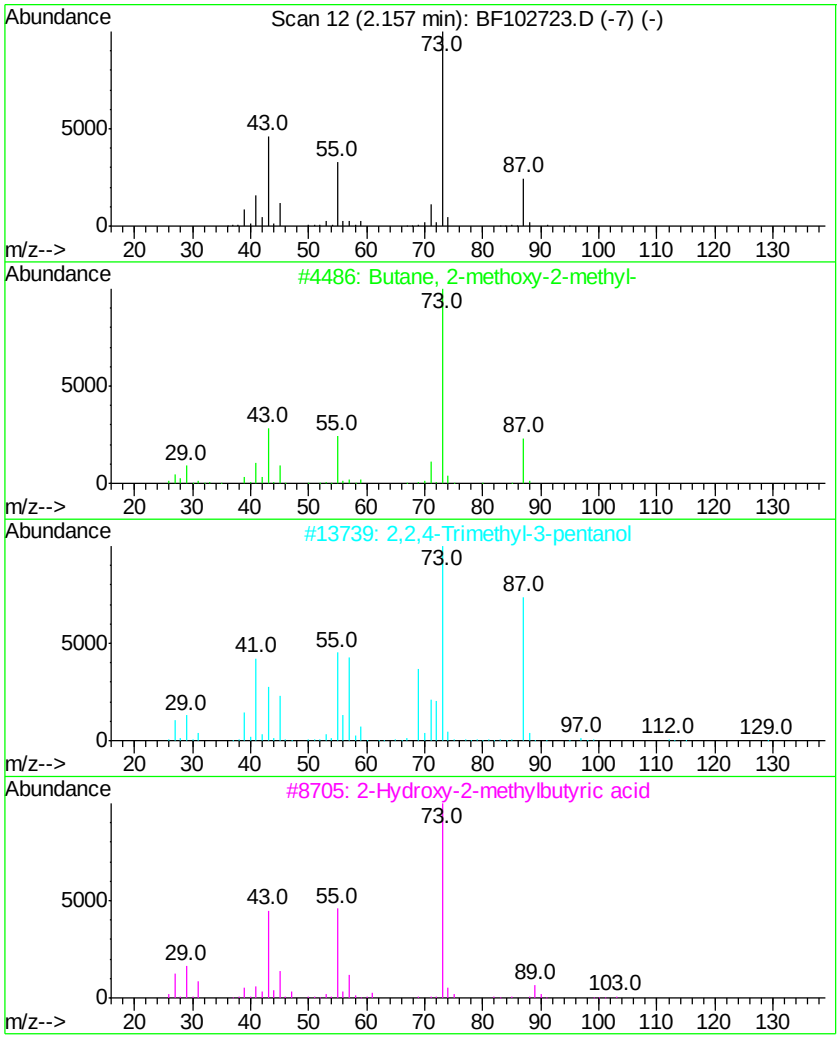
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

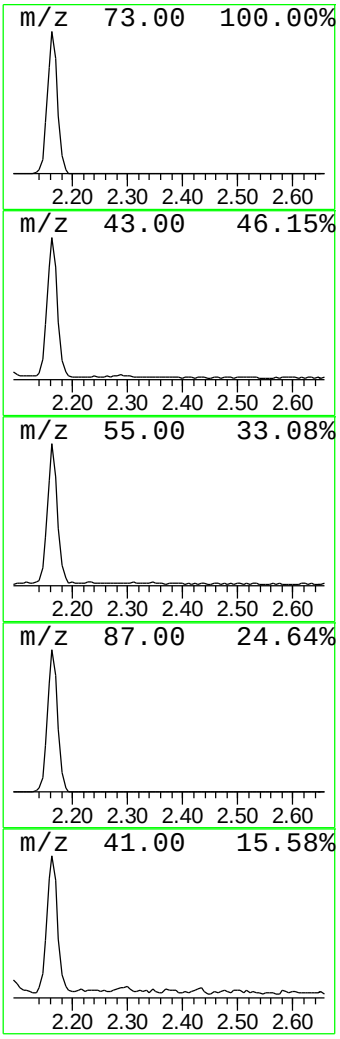
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	9.18 ng	546114	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	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	32
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23





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Data File : BF102723.D
Acq On : 3 Feb 2018 18:03
Operator : SJ/JU
Sample : J1436-17
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B25

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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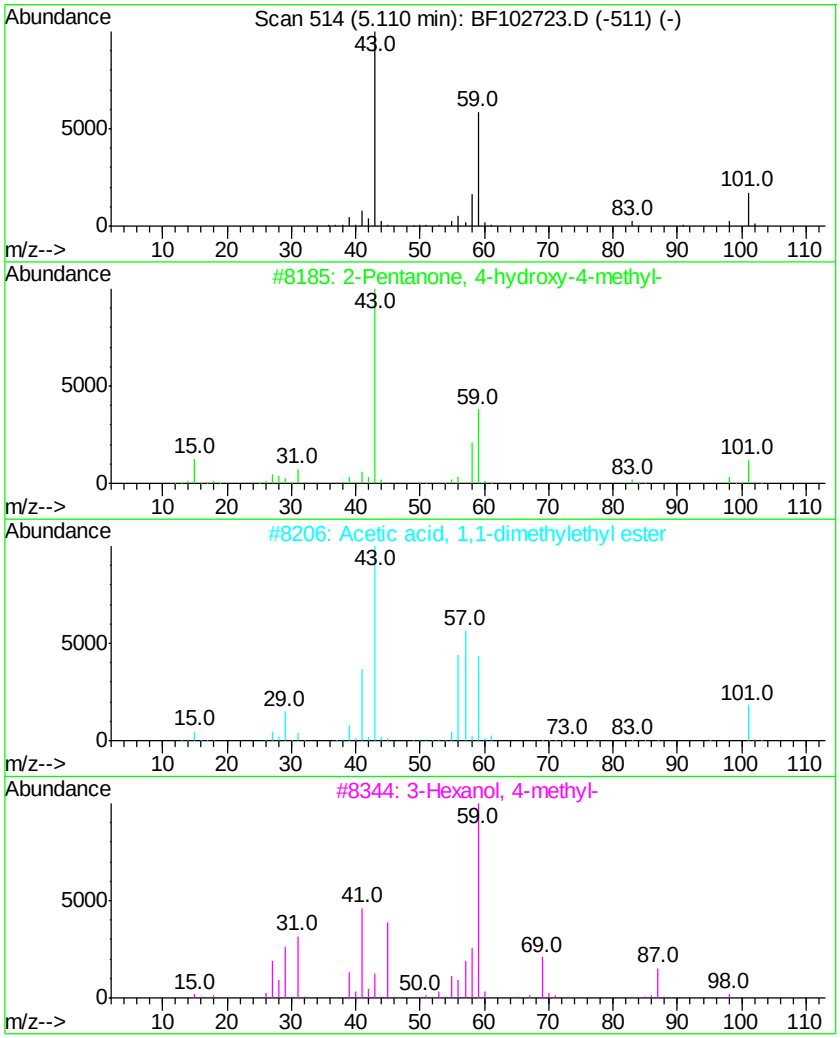
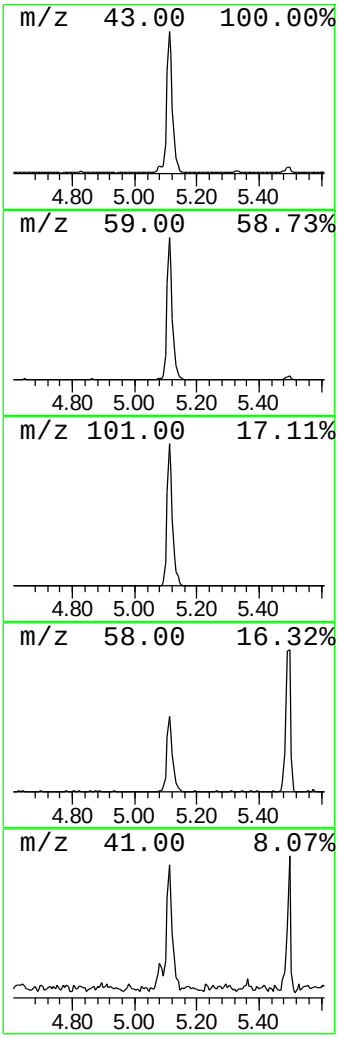
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	4.88 ng	290160	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	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Sample : J1436-17
Misc :
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Instrument : BNA_F
ClientSampleId : B25

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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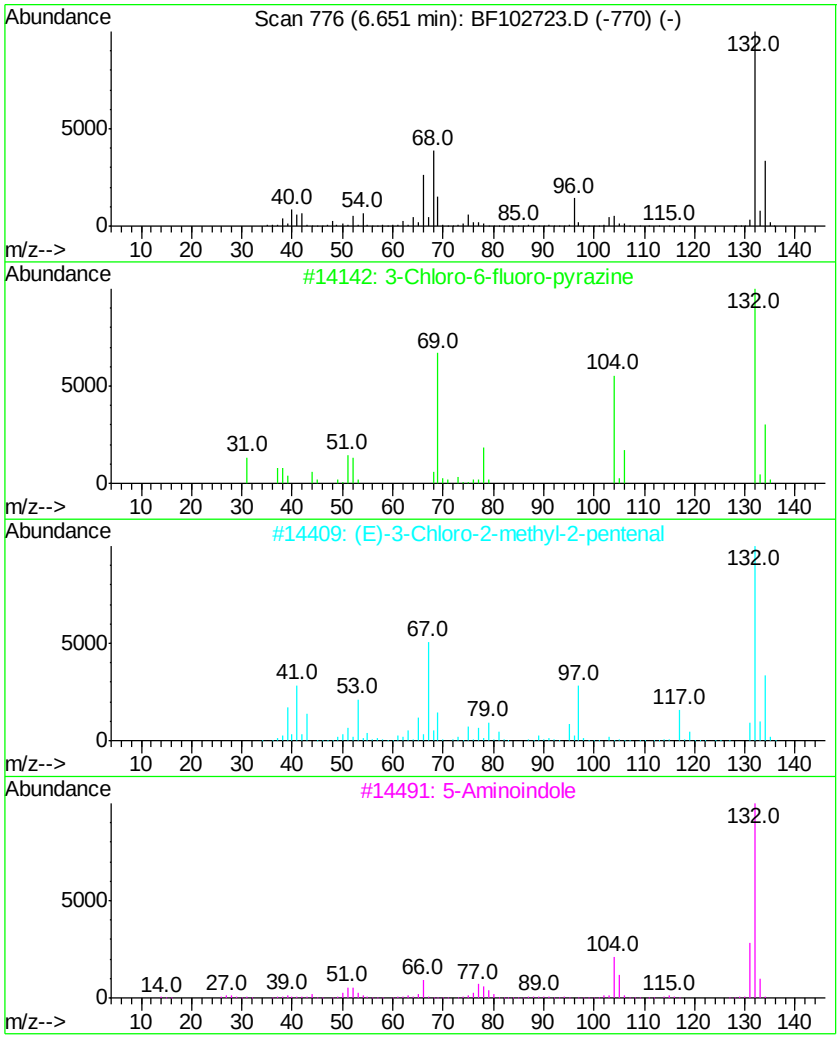
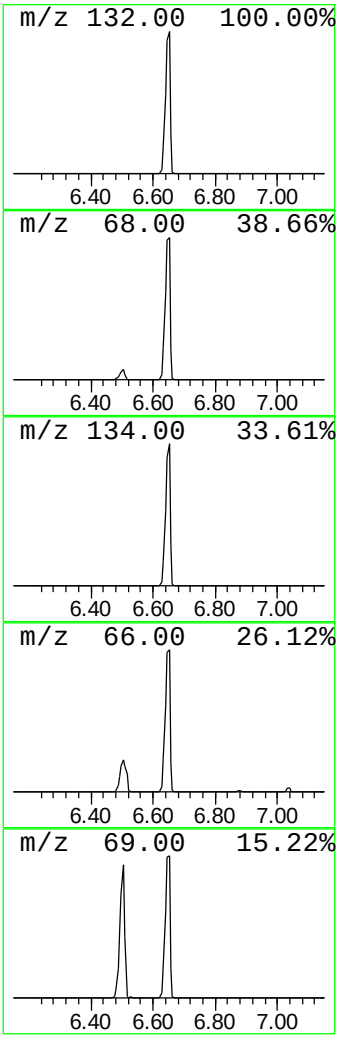
Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	79.30 ng	4719690	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	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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Operator : SJ/JU
Sample : J1436-17
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B25

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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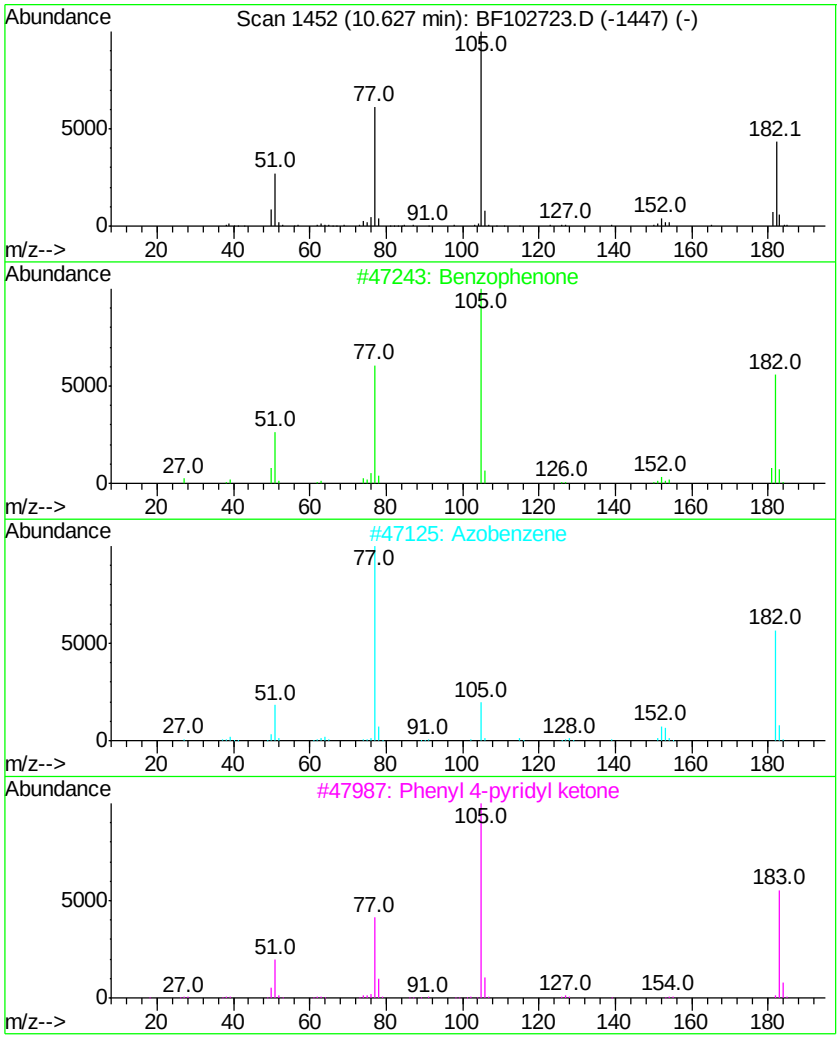
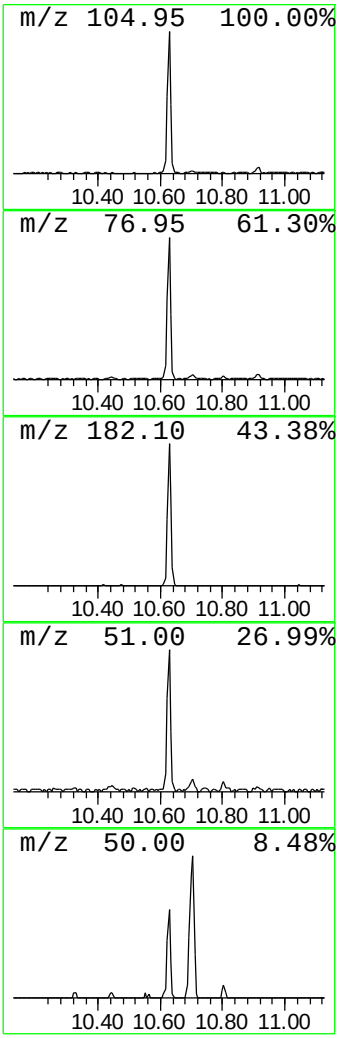
Peak Number 5 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	2.68 ng	221075	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	59
3	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	52
4	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
5	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47





Data Path : U:\HPCHEM1\BNA F\DATA\BF020318\
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Misc :
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Instrument : BNA_F
ClientSampleId : B25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
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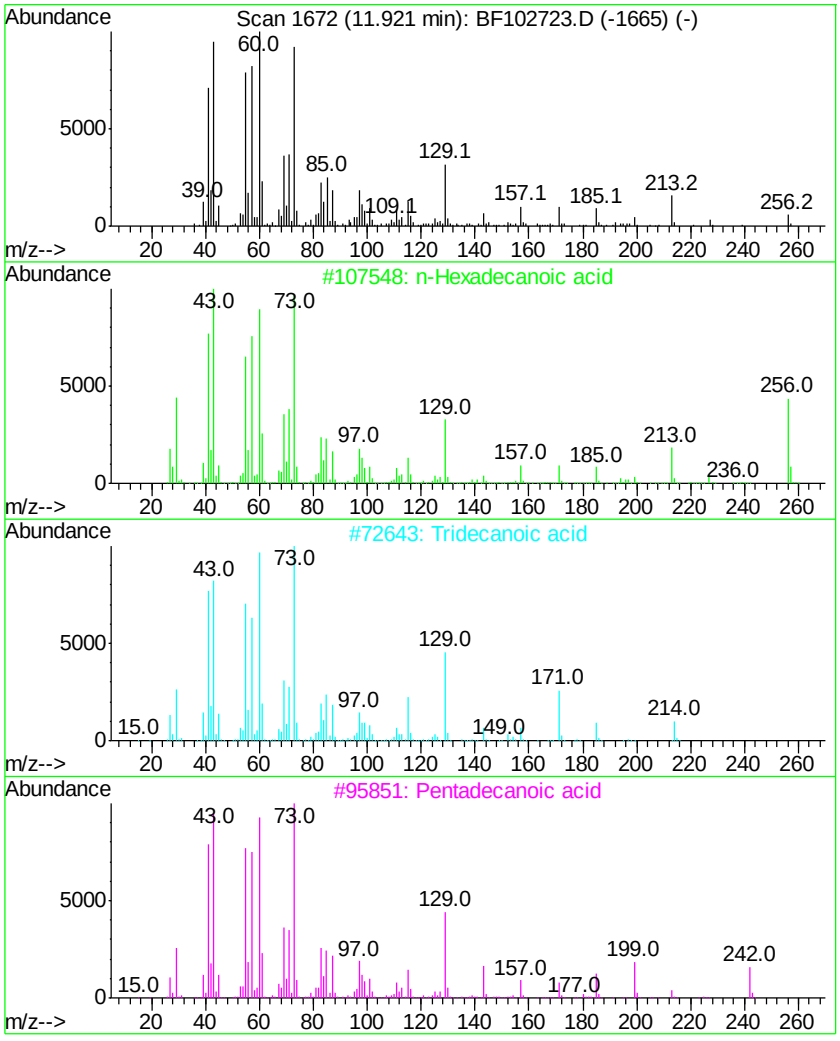
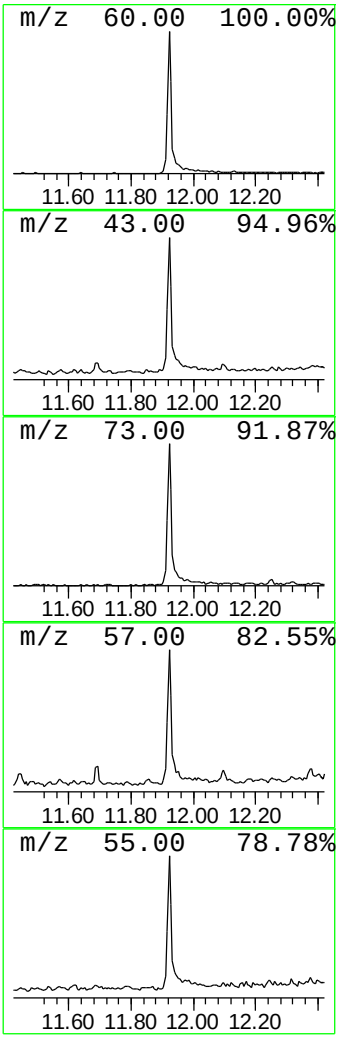
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	10.31 ng	689182	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	72





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Instrument : BNA_F
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TIC Library : C:\DATABASE\NIST11.L
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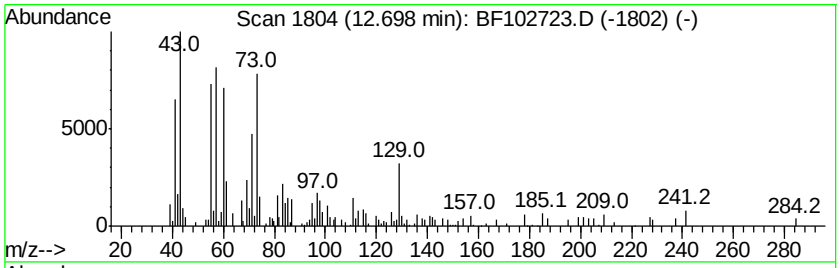
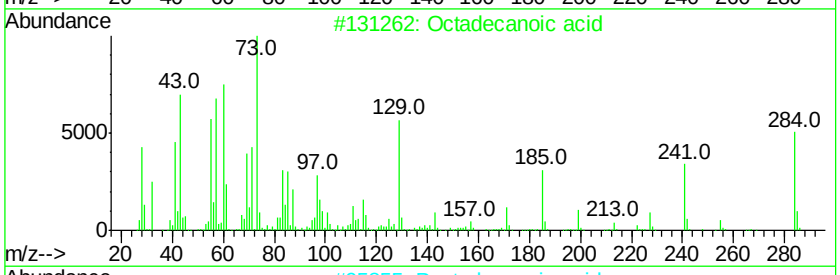
****

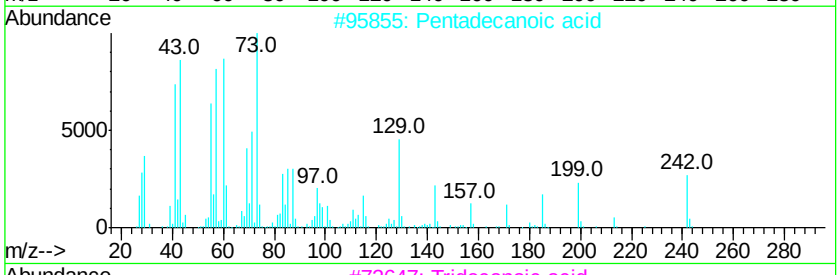
Peak Number 7 Octadecanoic acid Concentration Rank 7

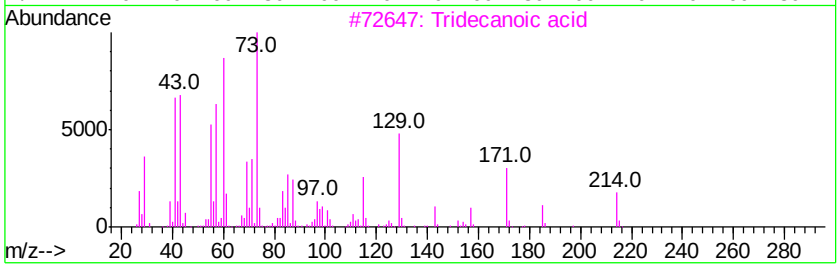
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	4.55 ng	303938	Phenanthrene-d10	11.40

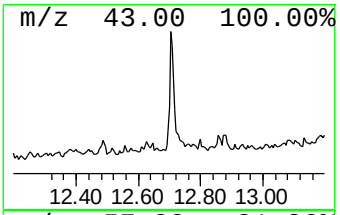
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80

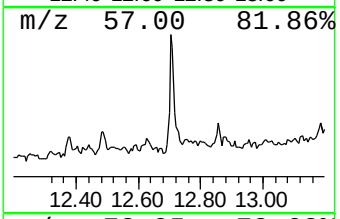


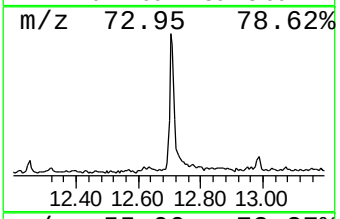


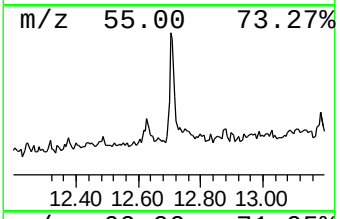


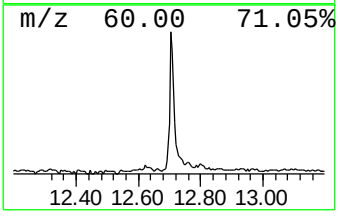












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

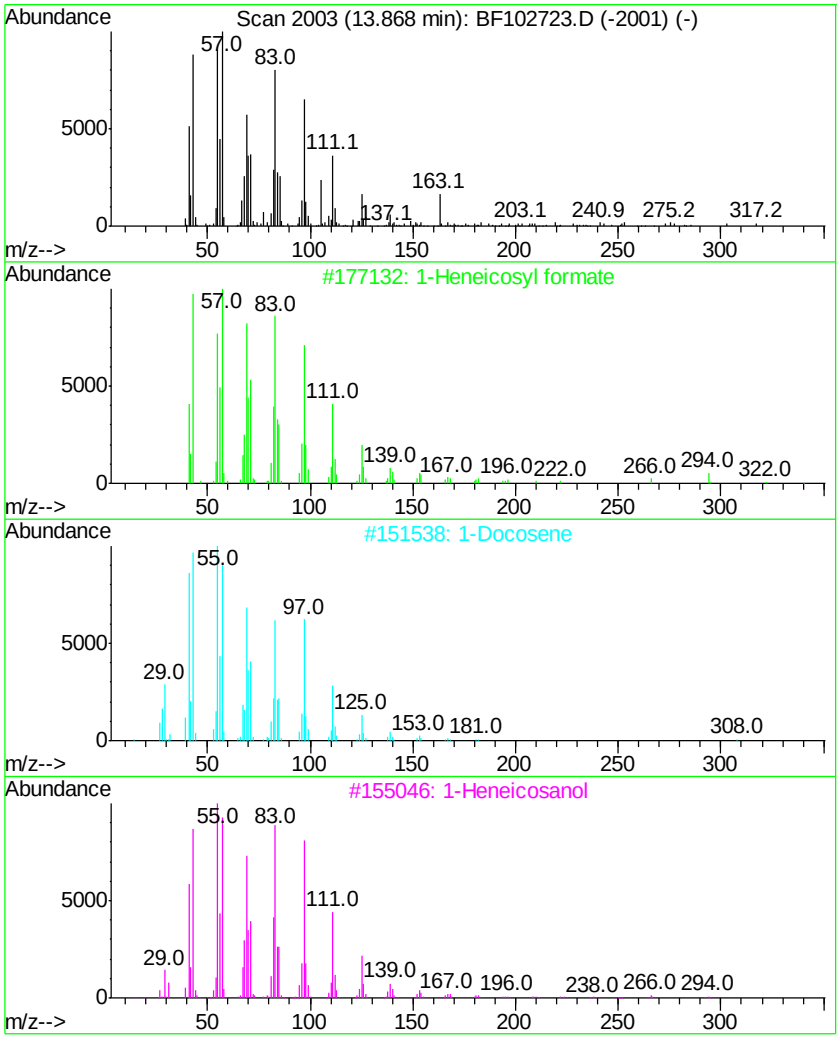
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

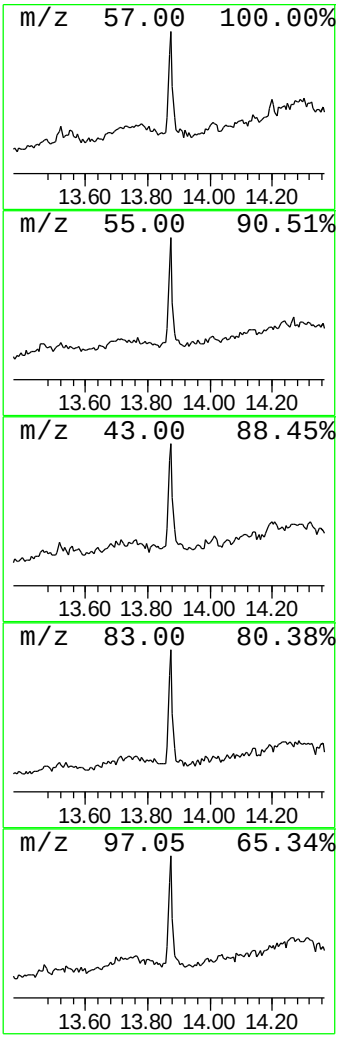
****

Peak Number 8 1-Heneicosyl formate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	6.73 ng	326542	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
2	1-Docosene	308	C22H44	001599-67-3	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	E-7-Octadecene	252	C18H36	1000130-92-0	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





Tentatively Identified Compound (LSC) summary

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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...	2.16	9.2	ng	546114	1	6.88	1190340	20.0
2-Pentanone, 4-hy...	5.11	4.9	ng	290160	1	6.88	1190340	20.0
unknown6.65	6.65	79.3	ng	4719690	1	6.88	1190340	20.0
Benzophenone	10.63	2.7	ng	221075	3	9.92	1647560	20.0
n-Hexadecanoic acid	11.92	10.3	ng	689182	4	11.40	1337200	20.0
Octadecanoic acid	12.70	4.5	ng	303938	4	11.40	1337200	20.0
1-Heneicosyl formate	13.87	6.7	ng	326542	5	14.04	970865	20.0