LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112717\
Data File : BF100895.D
Acq On : 27 Nov 2017 16:40
Operator : SJ/JU
Sample : I6513-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1

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-BF110817.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	3.987	309	323	326	rBV	4038122	8494030	100.00%	28.603%
2	5.104	509	513	523	rVB	106117	167412	1.97%	0.564%
3	5.492	574	579	588	rBV	2079307	2206044	25.97%	7.429%
4	6.498	744	750	762	rVB	1866690	2335649	27.50%	7.865%
5	6.634	768	773	776	rBV	2258014	2296768	27.04%	7.734%
6	6.857	807	811	815	rVB	660454	545947	6.43%	1.838%
7	7.016	834	838	841	rVB	1988372	1769987	20.84%	5.960%
8	7.428	902	908	910	rBV	1318231	1421311	16.73%	4.786%
9	8.139	1025	1029	1032	rVB	813790	656823	7.73%	2.212%
10	9.216	1206	1212	1215	rBV	2602985	2465107	29.02%	8.301%
11	9.604	1274	1278	1281	rBV	262903	199899	2.35%	0.673%
12	9.892	1323	1327	1331	rBV2	802044	706637	8.32%	2.380%
13	10.686	1457	1462	1465	rBV	1437863	1361147	16.02%	4.584%
14	11.380	1576	1580	1583	rBV	727944	593834	6.99%	2.000%
15	11.898	1663	1668	1679	rBV	449043	421962	4.97%	1.421%
16	12.680	1797	1801	1813	rBV	282331	305282	3.59%	1.028%
17	12.963	1845	1849	1853	rBV	1645873	1613657	19.00%	5.434%
18	13.845	1996	1999	2008	rVB	195591	206811	2.43%	0.696%
19	13.992	2020	2024	2026	rBV	849411	703363	8.28%	2.369%
20	14.021	2026	2029	2032	rVB	558963	502379	5.91%	1.692%
21	15.486	2273	2278	2287	rBV	420978	548780	6.46%	1.848%
22	15.986	2358	2363	2370	rVV3	47630	85001	1.00%	0.286%
23	17.115	2550	2555	2566	rBV7	39045	88210	1.04%	0.297%

Sum of corrected areas: 29696040

LSC Report - Integrated Chromatogram

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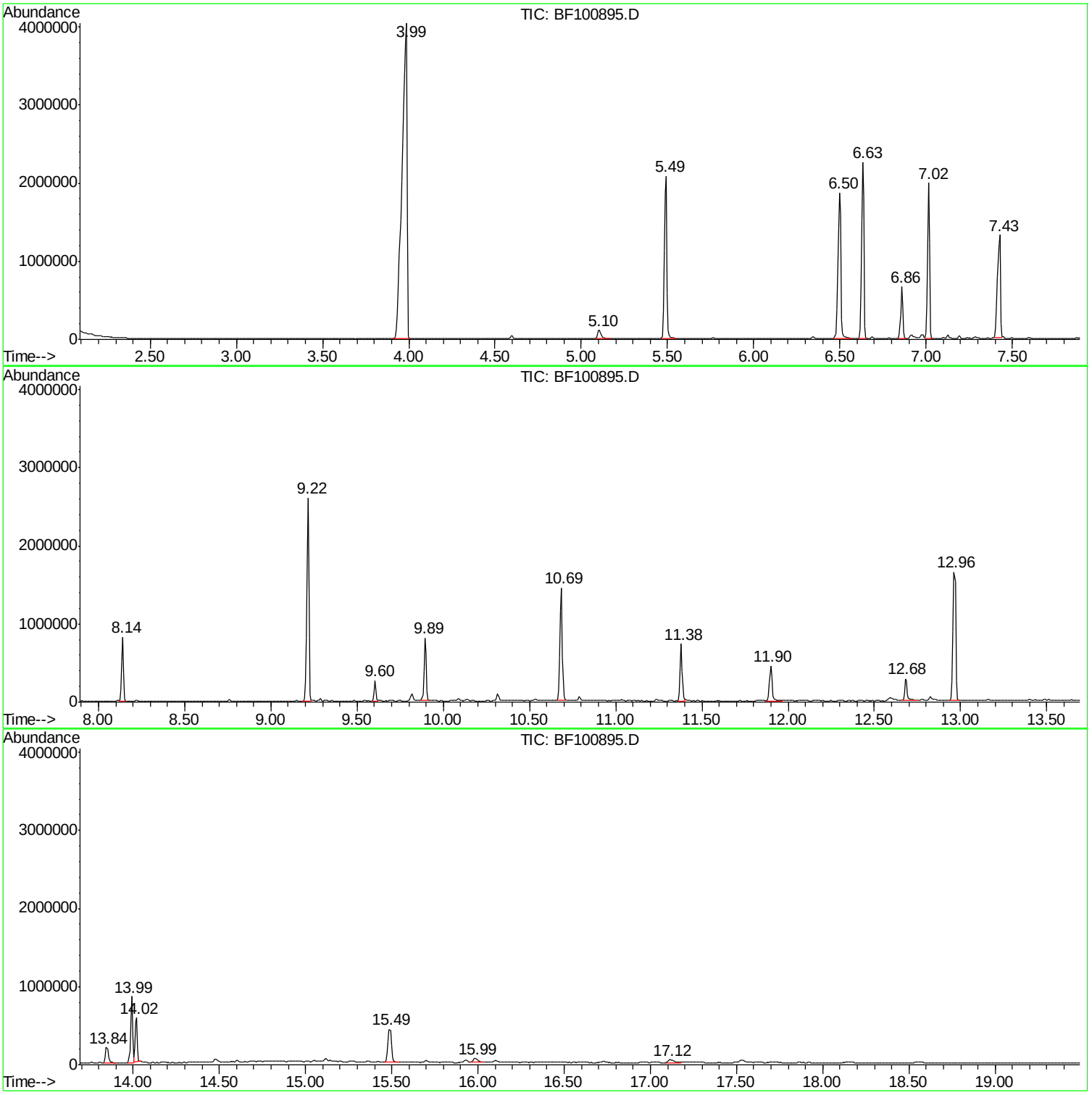
Operator : SJ/JU
Sample : I6513-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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

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Data File : BF100895.D
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Operator : SJ/JU
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Misc :
ALS Vial : 17 Sample Multiplier: 1

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ClientSampleId : SP-1

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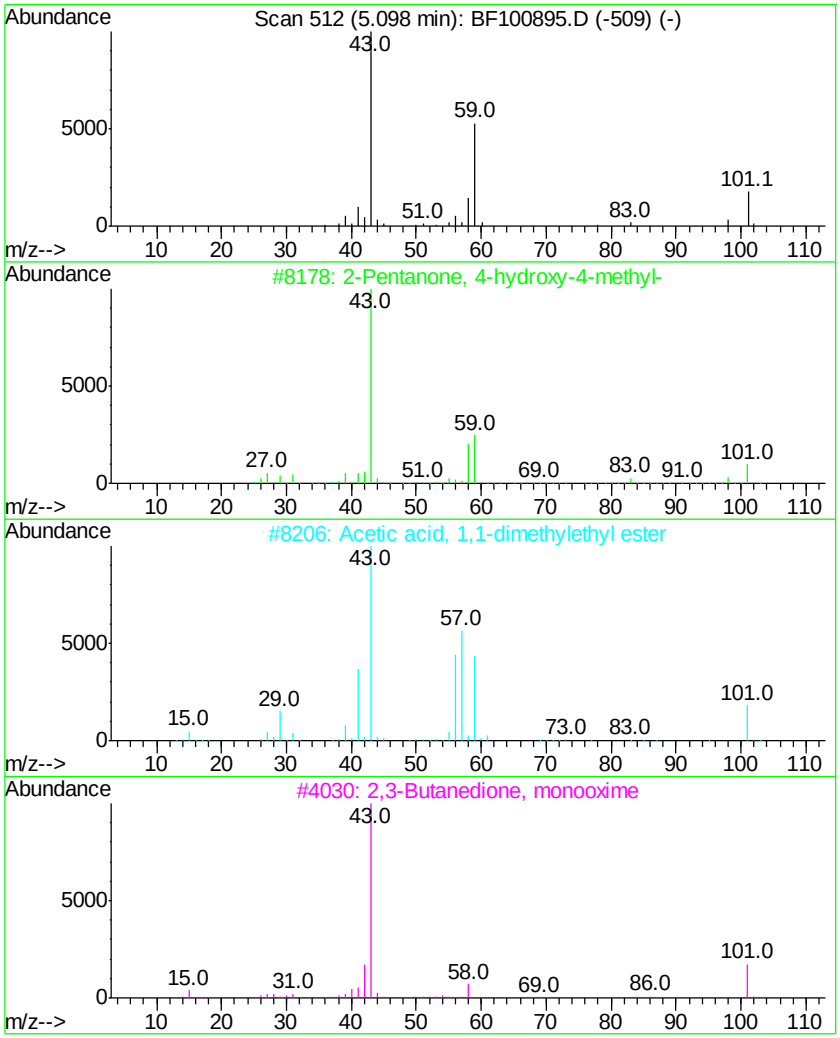
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

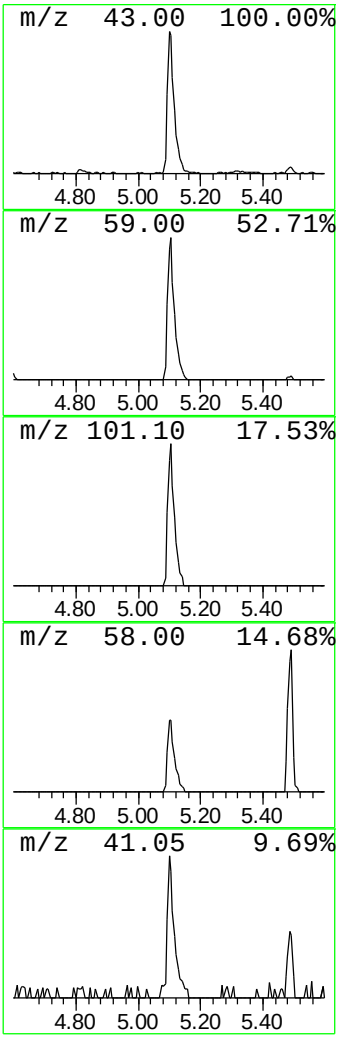
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	6.13 ng	167412	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28





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Operator : SJ/JU
Sample : I6513-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

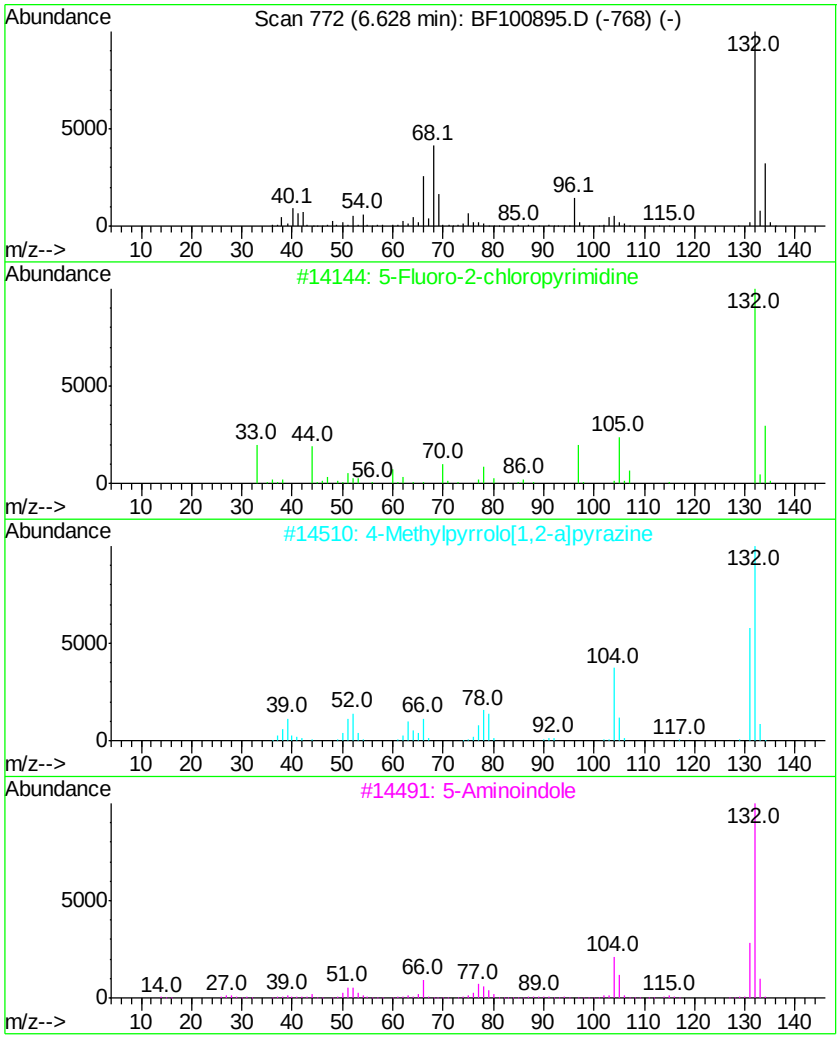
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

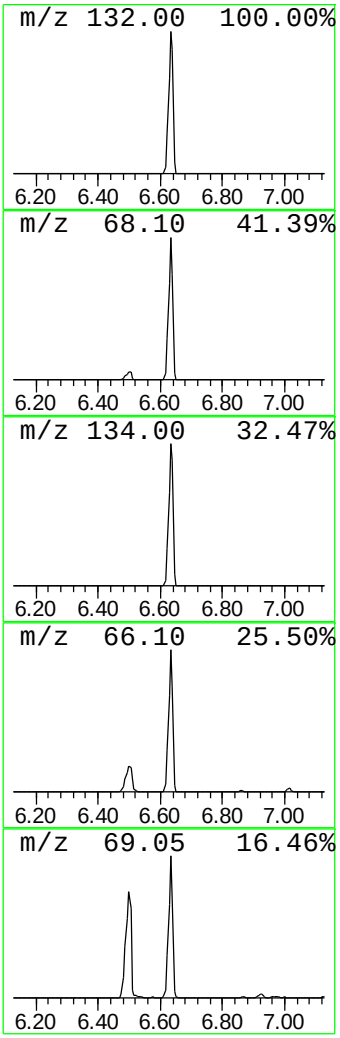
****

Peak Number 3 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	84.14 ng	2296770	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
2	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
3	5-Aminoindole	132	C8H8N2	005192-03-0	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Library Search Compound Report

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Acq On : 27 Nov 2017 16:40
Operator : SJ/JU
Sample : I6513-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

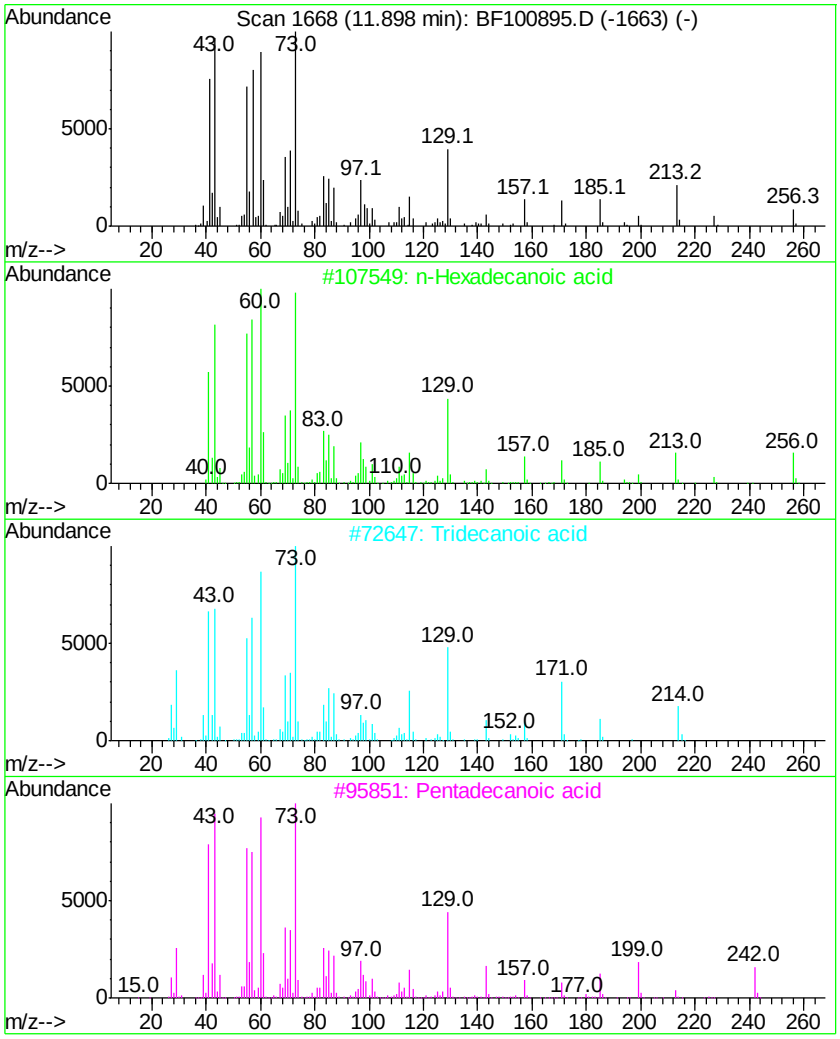
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

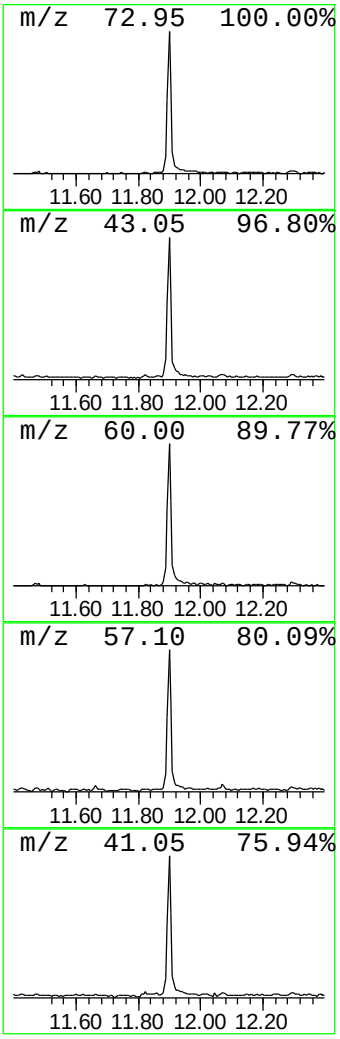
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	14.21 ng	421962	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	68





Library Search Compound Report

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Acq On : 27 Nov 2017 16:40
Operator : SJ/JU
Sample : I6513-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

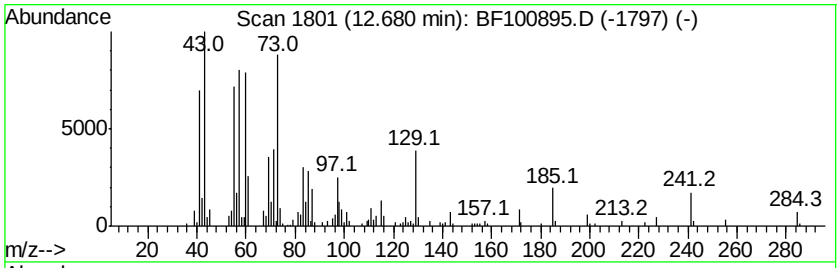
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

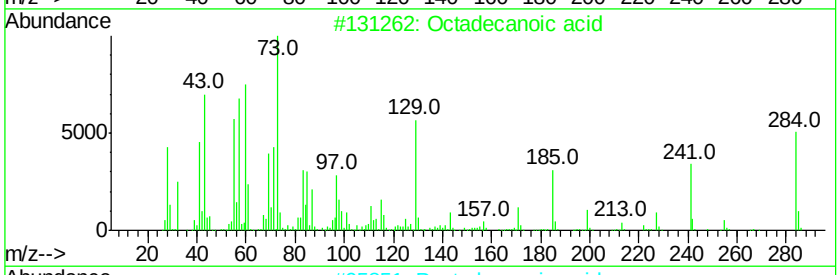
****

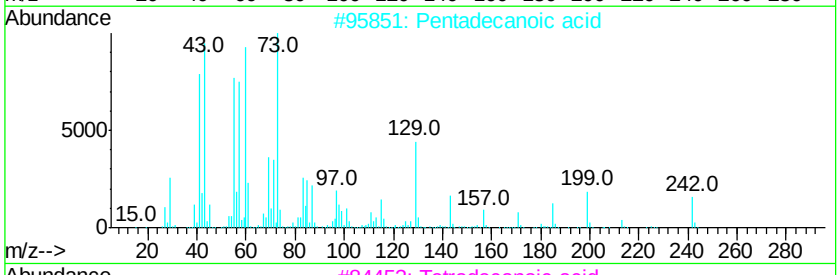
Peak Number 6 Octadecanoic acid Concentration Rank 5

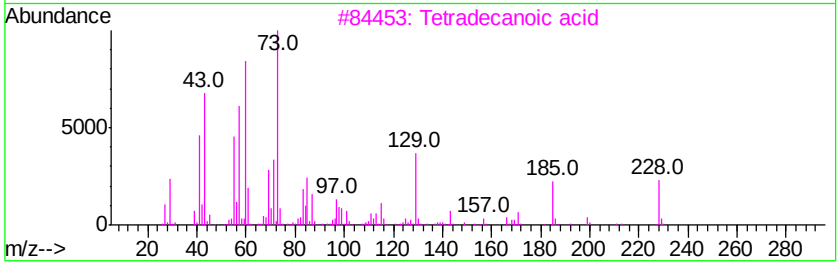
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.68	10.28 ng	305282	Phenanthrene-d10	11.38

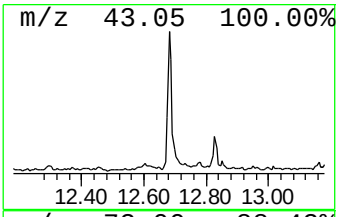
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70

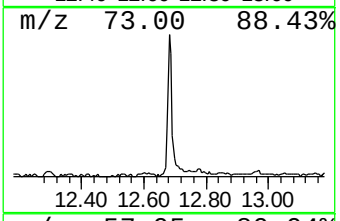


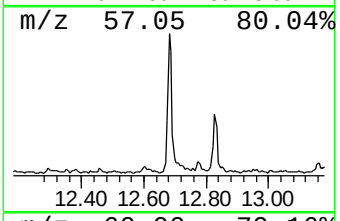


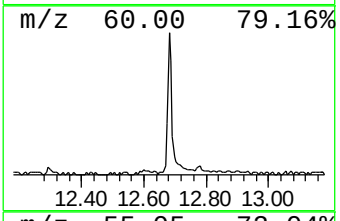


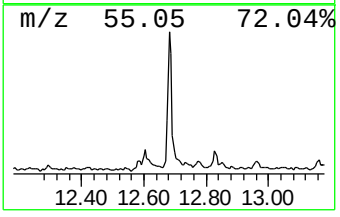












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Instrument : BNA_F
ClientSampleId : SP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

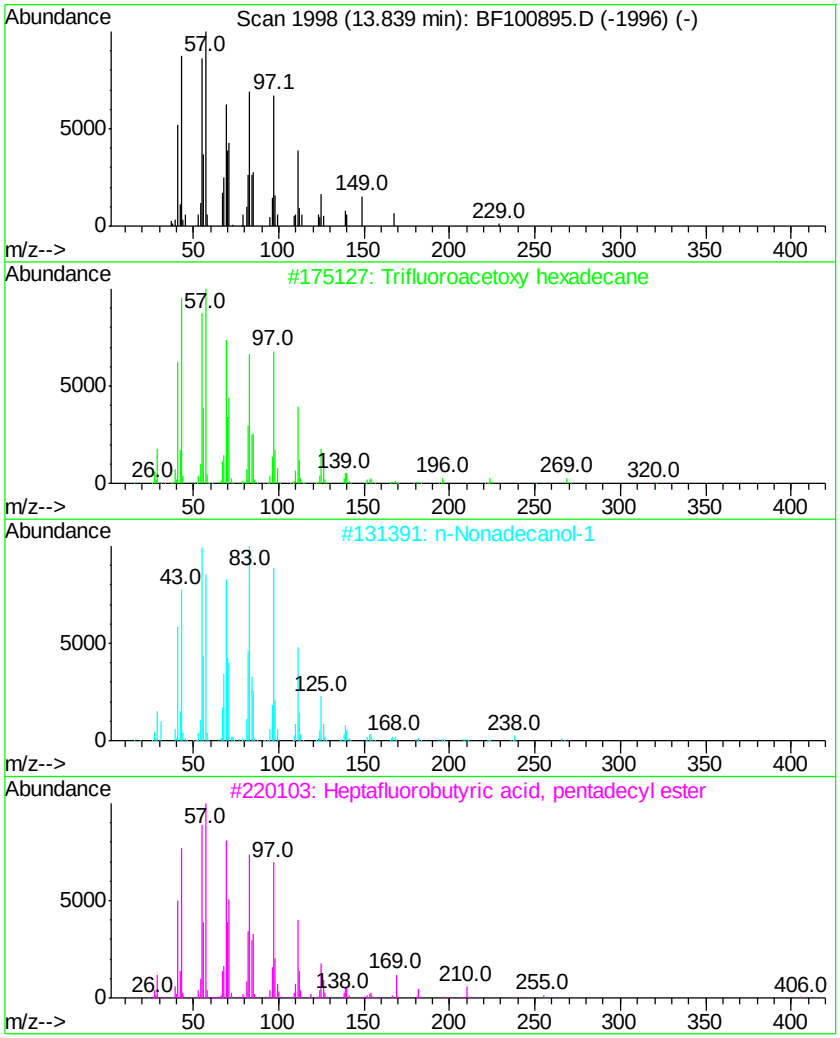
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

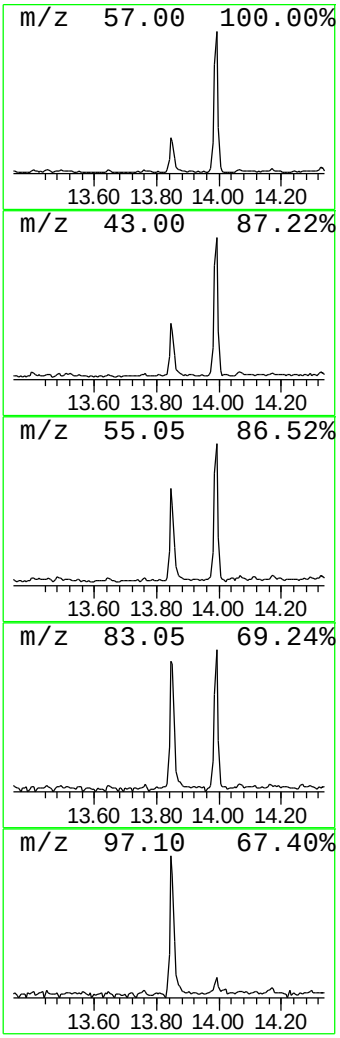
****

Peak Number 7 Trifluoroacetoxy hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	8.23 ng	206811	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
5	1-Heneicosanol	312	C21H44O	015594-90-8	95





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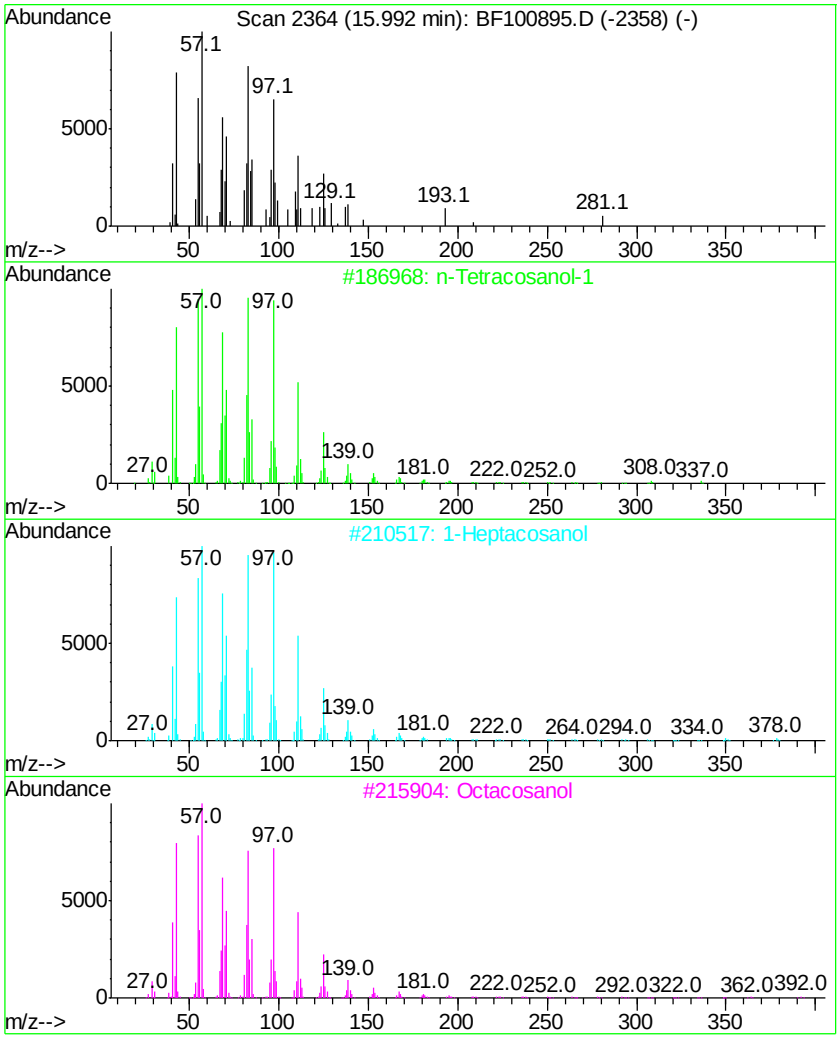
TIC Integration Parameters: LSCINT.P

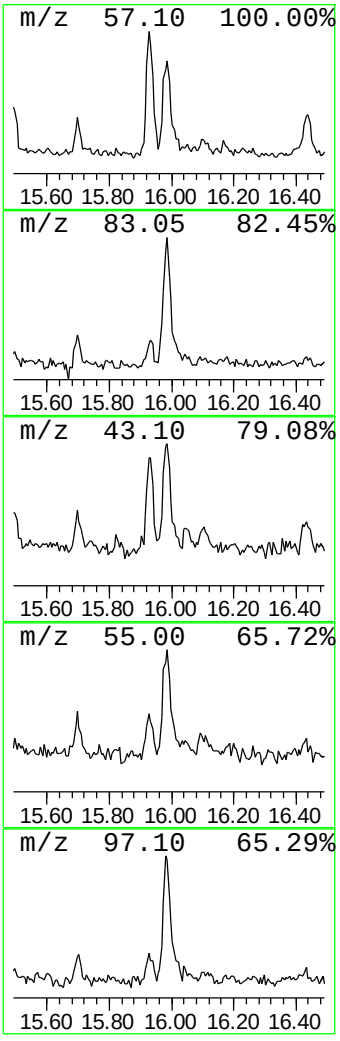
****

Peak Number 8 n-Tetracosanol-1 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.99	3.10 ng	85001	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2	1-Heptacosanol	396	C27H56O	002004-39-9	93
3	Octacosanol	410	C28H58O	000557-61-9	93
4	Heptacosyl acetate	438	C29H58O2	1000351-78-2	91
5	Behenic alcohol	326	C22H46O	000661-19-8	91





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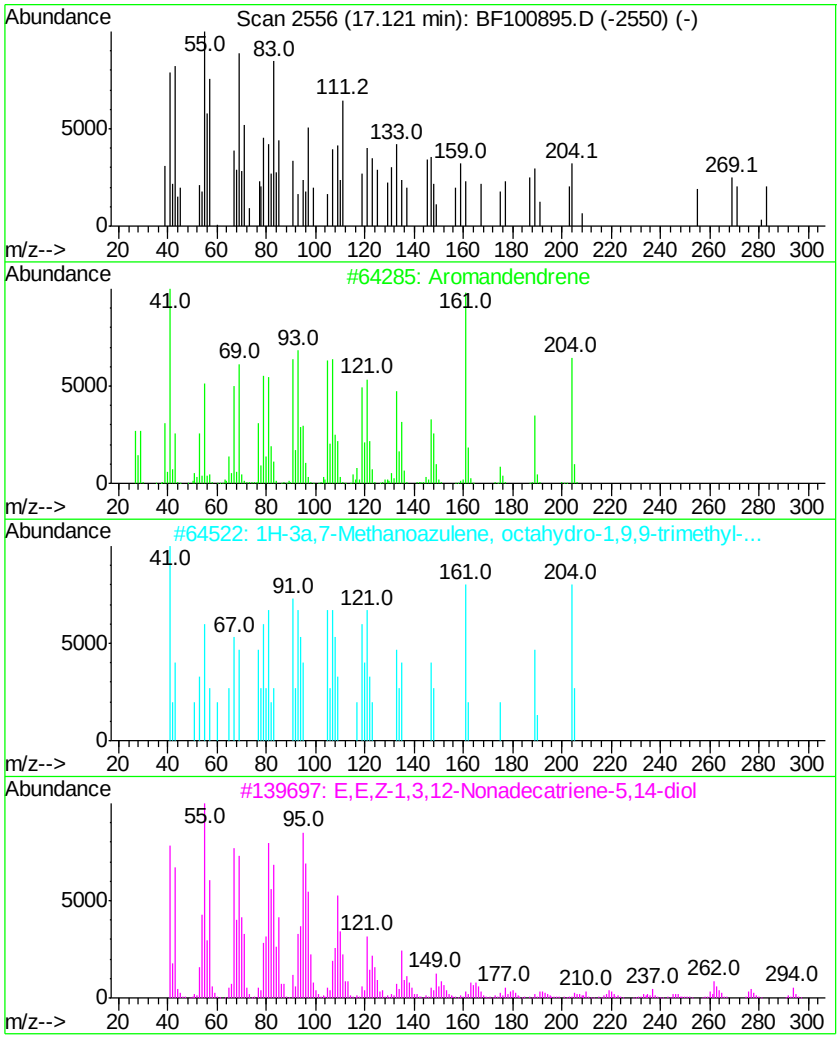
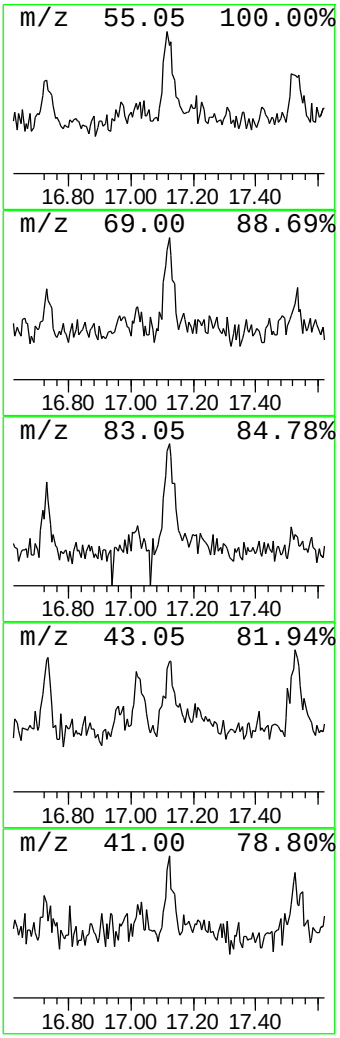
****

Peak Number 9 unknown17.12 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.12	3.21 ng	88210	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aromandendrene	204	C15H24	000489-39-4	47
2	1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	27
3	E,E,Z-1,3,12-Nonadecatriene-5,14...	294	C19H34O2	1000131-11-4	22
4	Isobutyl tridecyl carbonate	300	C18H36O3	959275-44-6	15
5	Dichloroacetic acid, 2-pentadecy...	338	C17H32Cl2O2	1000280-64-7	11





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.10	6.1	ng	167412	1	6.86	545947	20.0
unknown6.63	6.63	84.1	ng	2296770	1	6.86	545947	20.0
n-Hexadecanoic acid	11.90	14.2	ng	421962	4	11.38	593834	20.0
Octadecanoic acid	12.68	10.3	ng	305282	4	11.38	593834	20.0
Trifluoroacetoxy ...	13.84	8.2	ng	206811	5	14.02	502379	20.0
n-Tetracosanol-1	15.99	3.1	ng	85001	6	15.49	548780	20.0
unknown17.12	17.12	3.2	ng	88210	6	15.49	548780	20.0