LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102894.D
Acq On : 9 Feb 2018 17:43
Operator : SJ/JU
Sample : PB106115BL
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB106115BL

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	2.204	11	20	27	rVB	149384	229652	5.57%	0.690%
2	5.122	509	516	524	rBV	110145	146700	3.56%	0.441%
3	5.510	577	582	585	rBV	4190186	4126161	100.00%	12.397%
4	6.510	747	752	755	rBV	3556525	3878838	94.01%	11.654%
5	6.657	772	777	780	rBV	3924663	3948062	95.68%	11.862%
6	6.886	812	816	819	rBV	1084727	977820	23.70%	2.938%
7	7.039	838	842	846	rBV	3327657	3119281	75.60%	9.372%
8	7.445	906	911	914	rBV	2624451	2641601	64.02%	7.937%
9	8.169	1029	1034	1037	rBV	1422745	1246046	30.20%	3.744%
10	9.245	1211	1217	1220	rBV	3884452	3917107	94.93%	11.769%
11	9.921	1328	1332	1342	rBV2	1283262	1193247	28.92%	3.585%
12	10.716	1462	1467	1478	rBV	1703516	1842876	44.66%	5.537%
13	11.410	1582	1585	1597	rBV	1016668	948008	22.98%	2.848%
14	12.810	1820	1823	1826	rBV	128695	105295	2.55%	0.316%
15	12.998	1850	1855	1858	rBV	2929068	2756531	66.81%	8.282%
16	13.515	1940	1943	1948	rBV2	91911	86672	2.10%	0.260%
17	14.051	2030	2034	2044	rBV	855298	863515	20.93%	2.594%
18	15.162	2219	2223	2227	rBV2	46669	54819	1.33%	0.165%
19	15.539	2282	2287	2298	rBV	614359	878679	21.30%	2.640%
20	15.998	2360	2365	2369	rBV2	58199	85790	2.08%	0.258%
21	16.515	2447	2453	2460	rBV2	69581	132303	3.21%	0.397%
22	17.121	2552	2556	2565	rVB2	50252	104875	2.54%	0.315%

Sum of corrected areas: 33283878

LSC Report - Integrated Chromatogram

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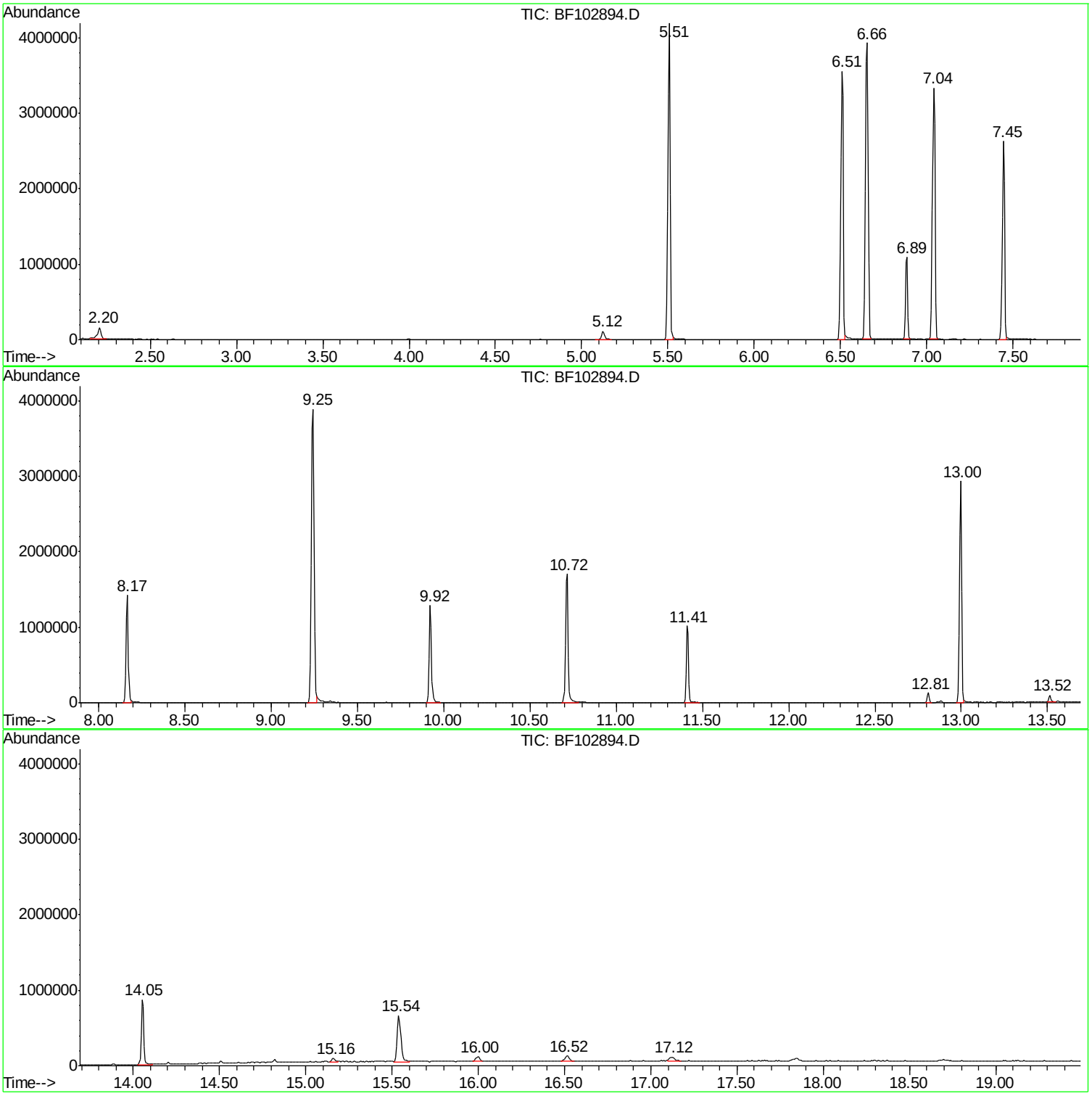
Data File : BF102894.D
Acq On : 9 Feb 2018 17:43
Operator : SJ/JU
Sample : PB106115BL
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB106115BL

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102894.D
Acq On : 9 Feb 2018 17:43
Operator : SJ/JU
Sample : PB106115BL
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB106115BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

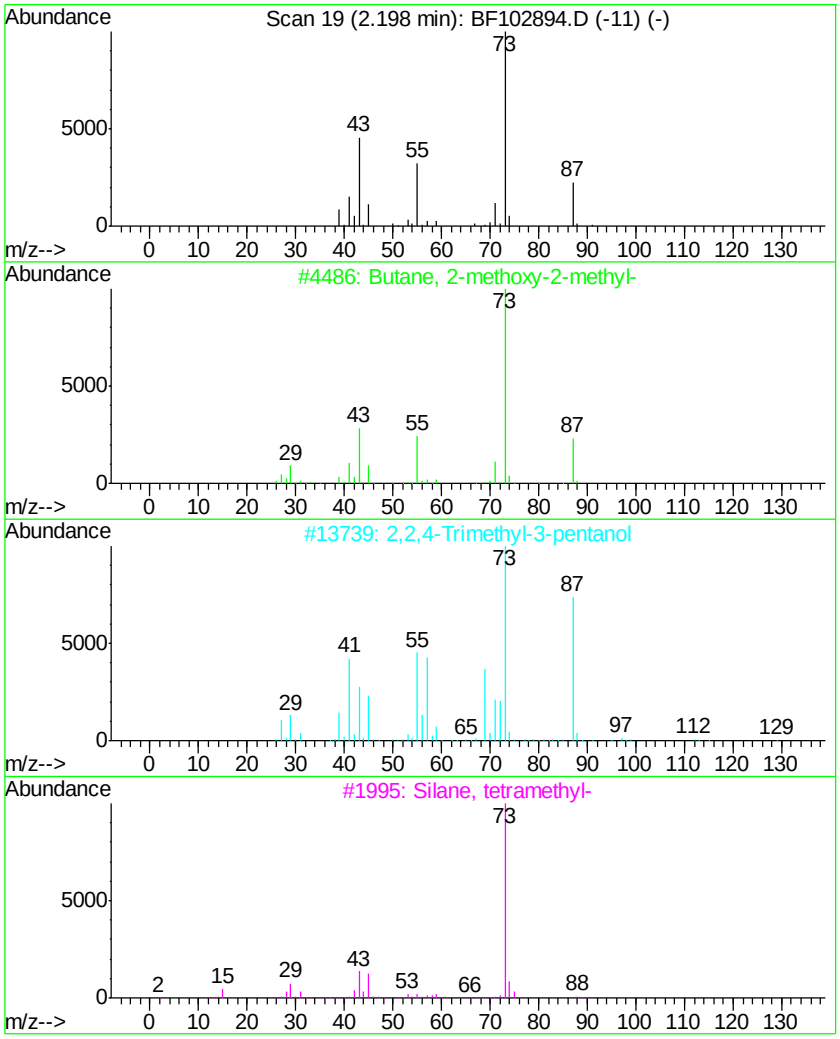
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

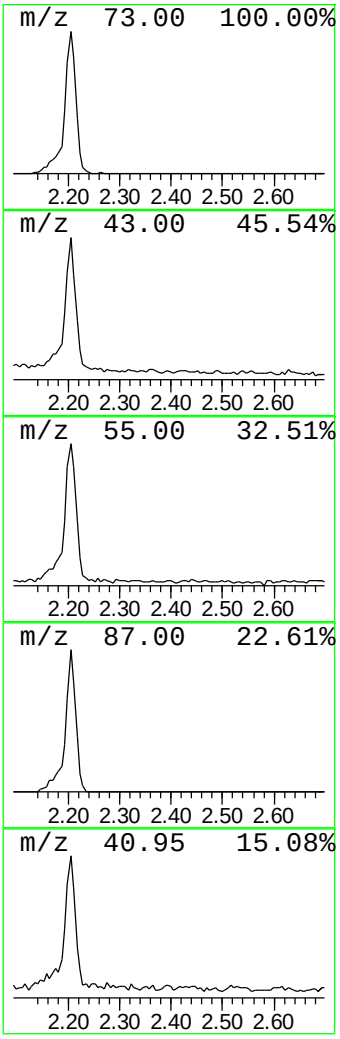
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	4.70 ng	229652	1,4-Dichlorobenzene-d4	6.89

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	23
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	17
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	17





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102894.D
Acq On : 9 Feb 2018 17:43
Operator : SJ/JU
Sample : PB106115BL
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB106115BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

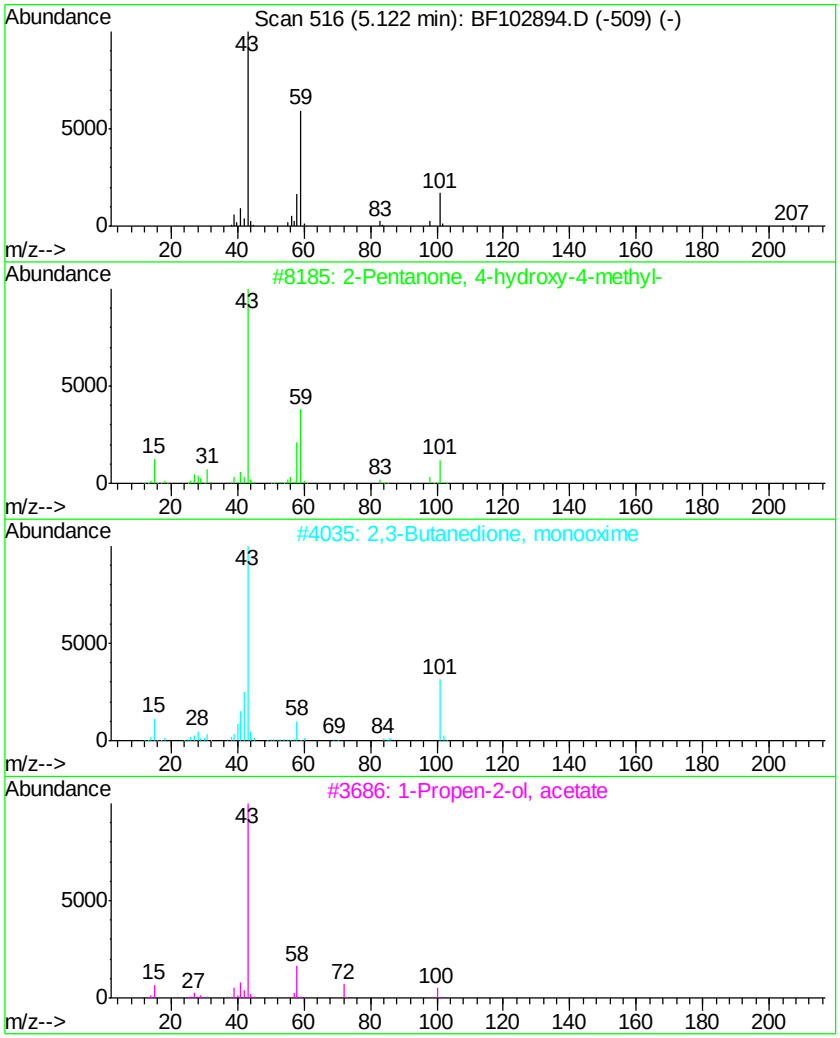
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

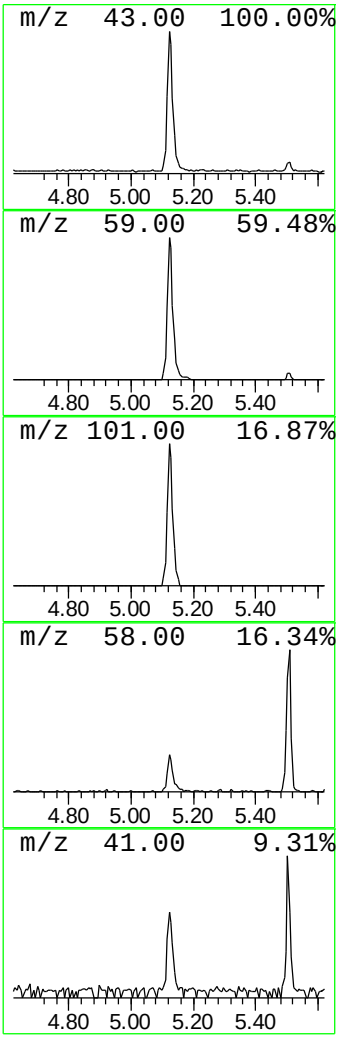
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	3.00 ng	146700	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	14
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4	.alpha.-Hydroxyisobutyric acid, ...	146	C6H10O4	1000374-31-3	9
5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9





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Data File : BF102894.D
Acq On : 9 Feb 2018 17:43
Operator : SJ/JU
Sample : PB106115BL
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB106115BL

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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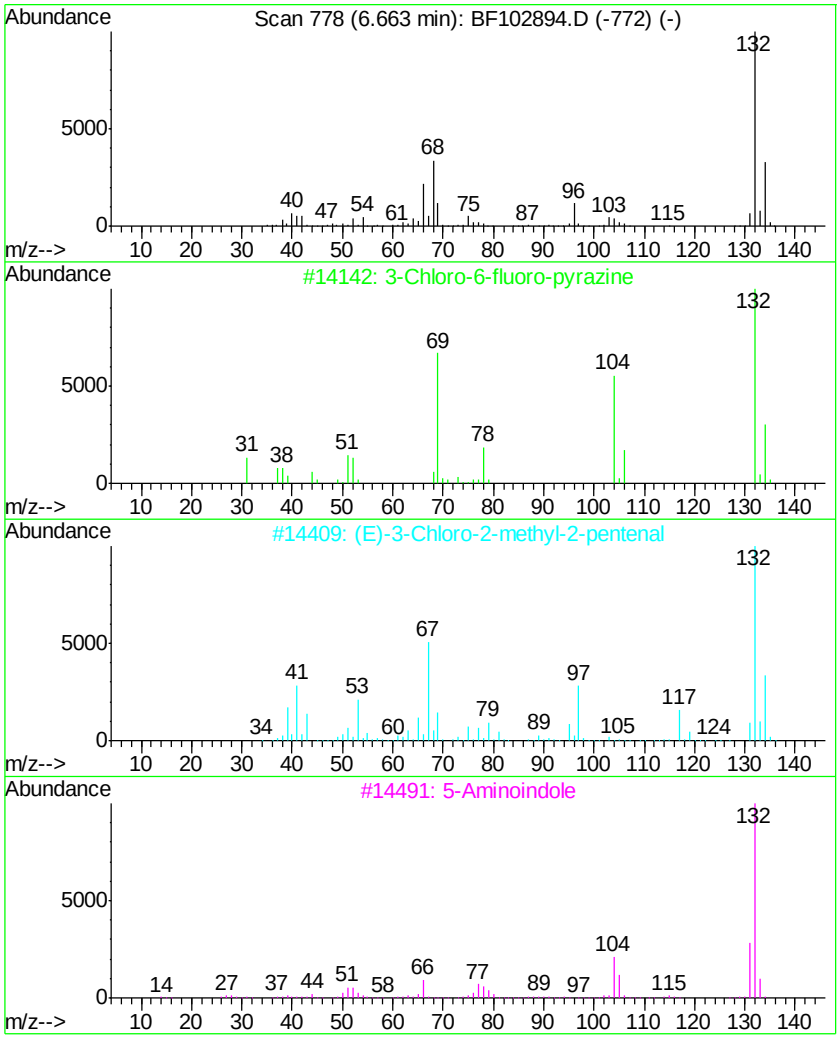
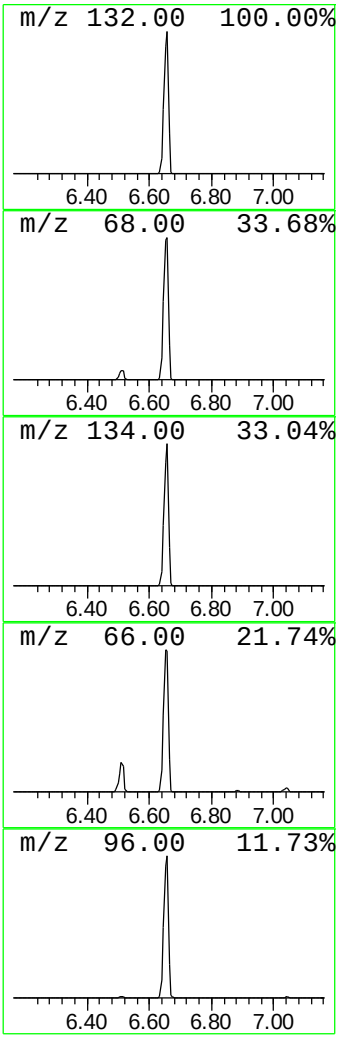
Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	80.75 ng	3948060	1,4-Dichlorobenzene-d4	6.89

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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102894.D
Acq On : 9 Feb 2018 17:43
Operator : SJ/JU
Sample : PB106115BL
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB106115BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

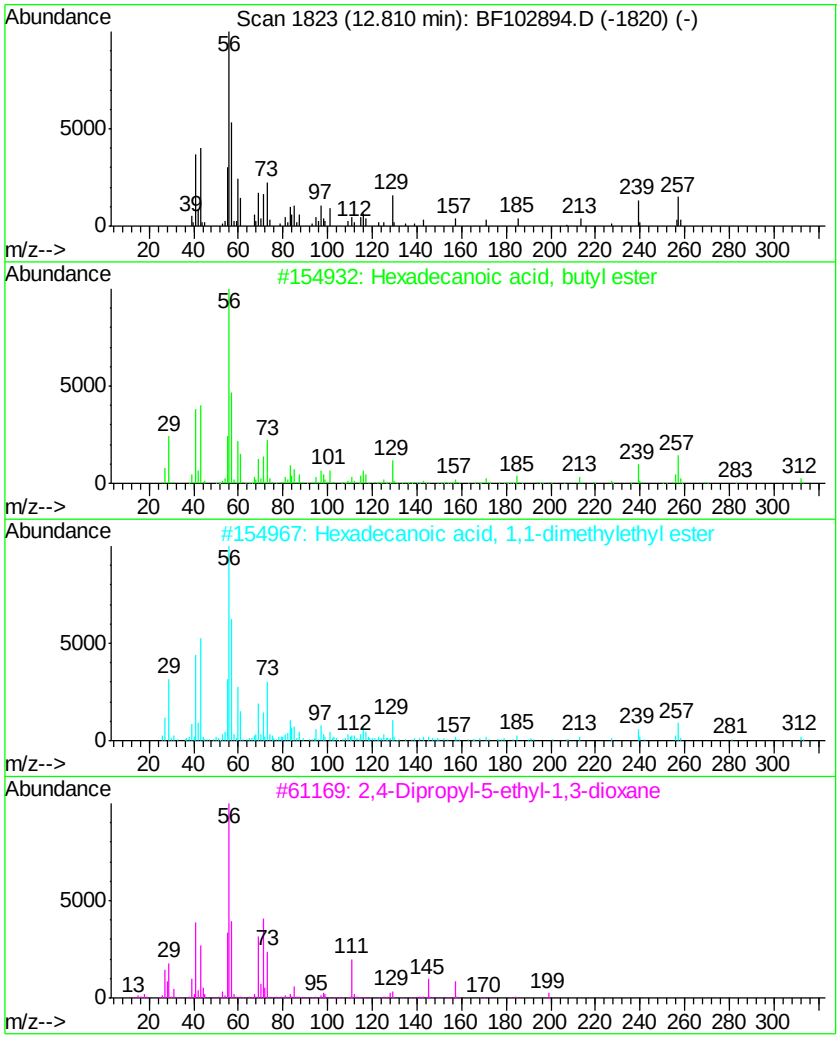
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

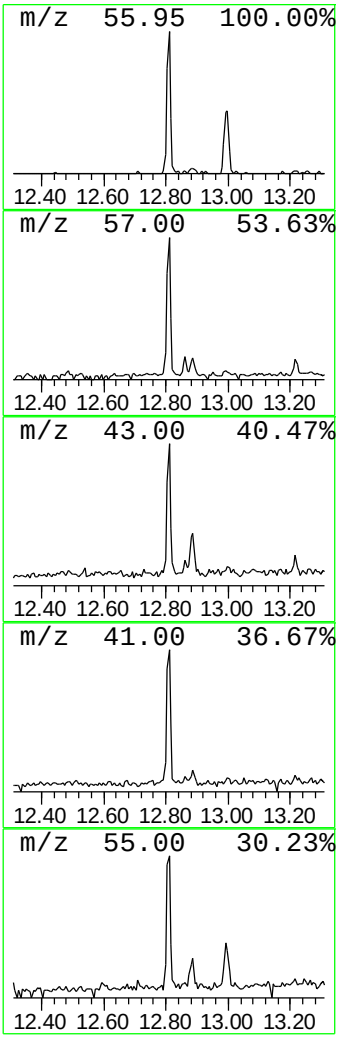
****

Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.81	2.44 ng	105295	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	87
3	2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	38
4	1-Pentadecene, 2-methyl-	224	C16H32	029833-69-0	32
5	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	32





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Sample : PB106115BL
Misc :
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Instrument : BNA_F
ClientSampleId : PB106115BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

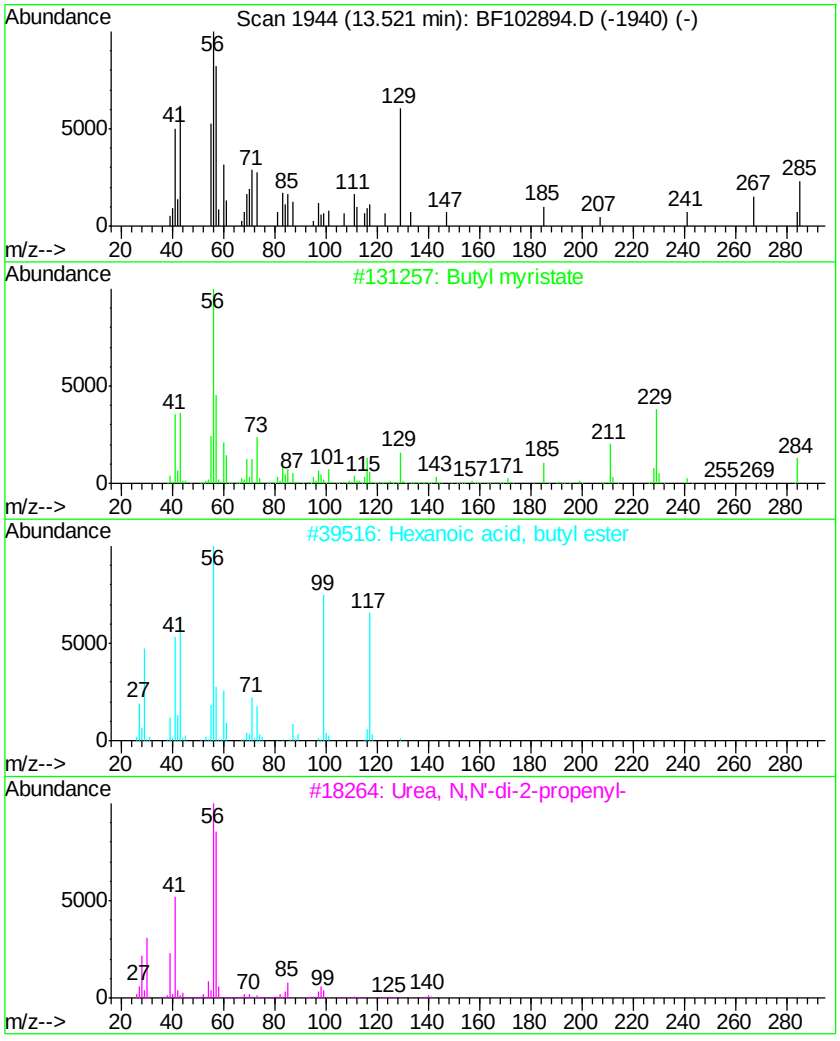
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

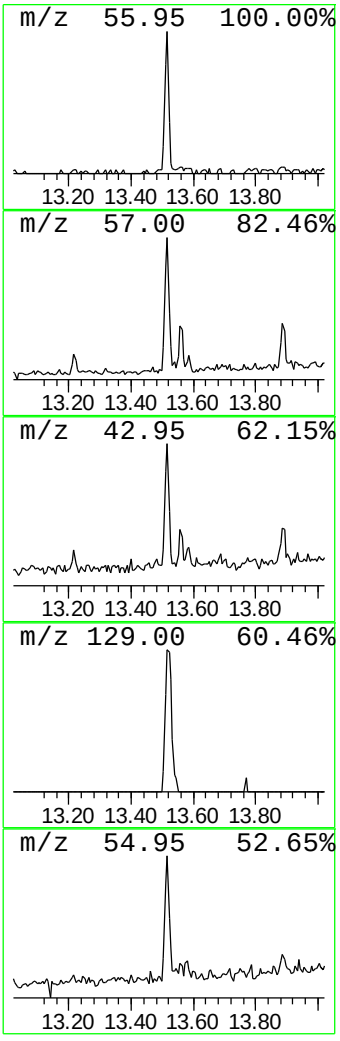
****

Peak Number 6 Butyl myristate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.52	2.01 ng	86672	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	64
2	Hexanoic acid, butyl ester	172	C10H20O2	000626-82-4	50
3	Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	38
4	Cyclopentanone, 2,2-dimethyl-	112	C7H12O	004541-32-6	38
5	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	38





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Misc :
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Instrument : BNA_F
ClientSampleId : PB106115BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

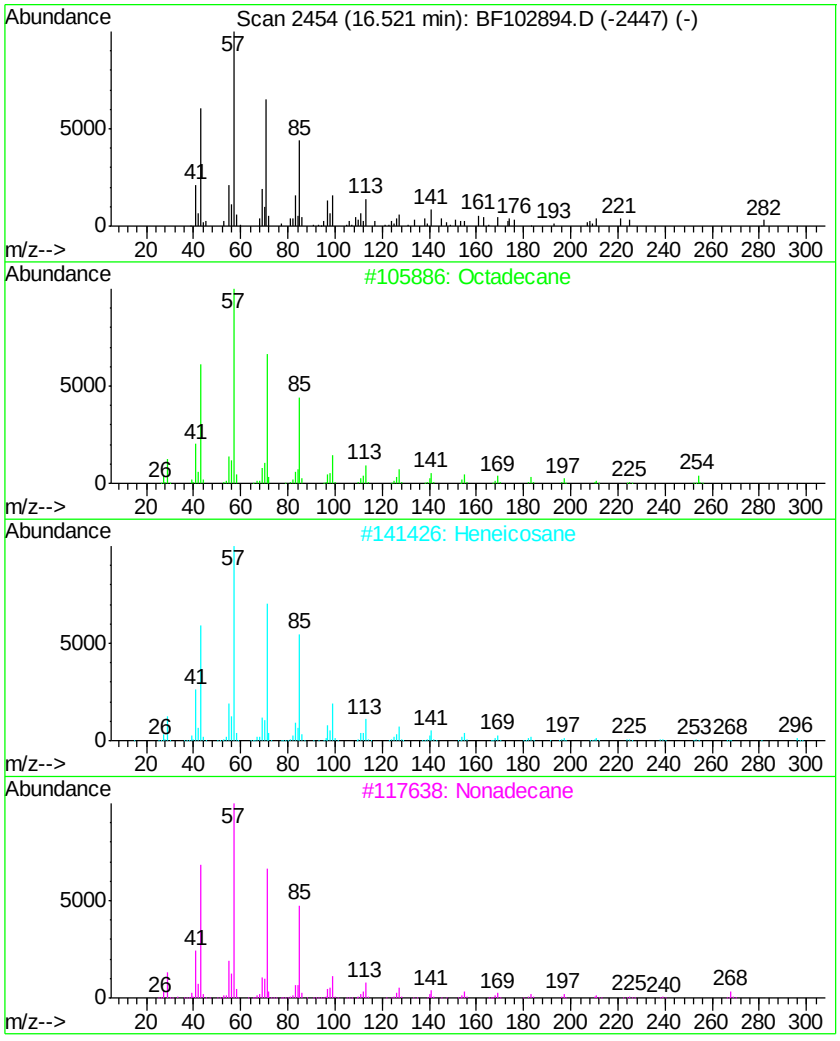
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

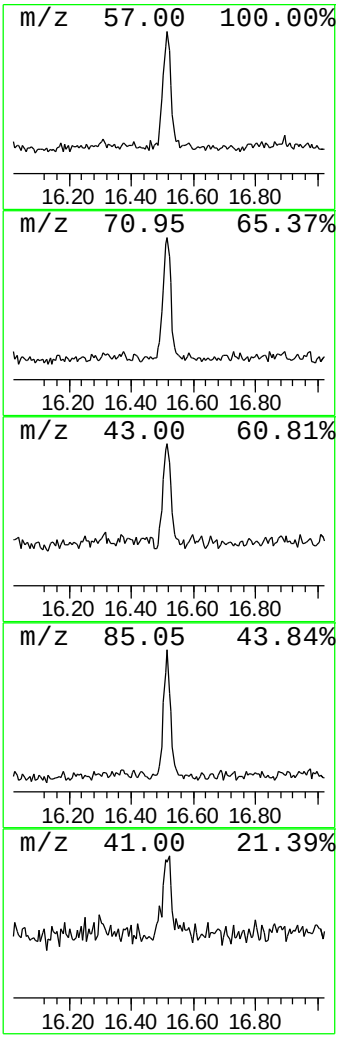
****

Peak Number 7 Octadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.52	3.01 ng	132303	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	91
2	Heneicosane	296	C21H44	000629-94-7	87
3	Nonadecane	268	C19H40	000629-92-5	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Eicosane	282	C20H42	000112-95-8	86





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Misc :
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Instrument : BNA_F
ClientSampleId : PB106115BL

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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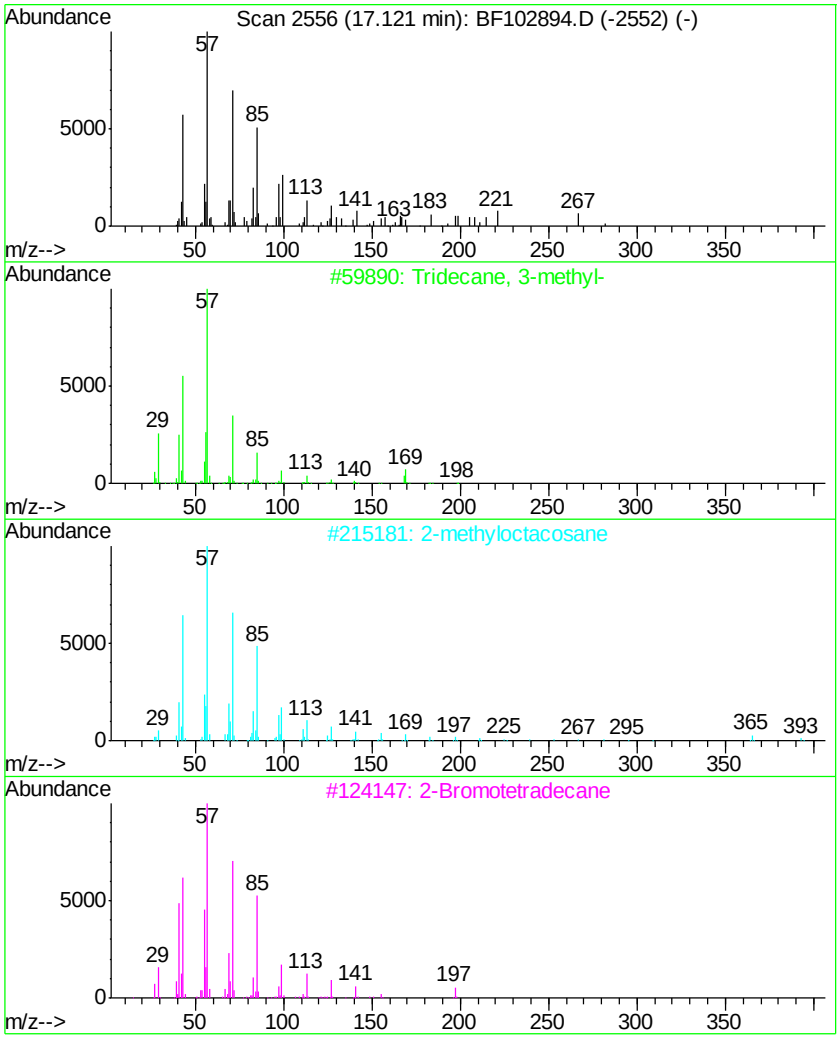
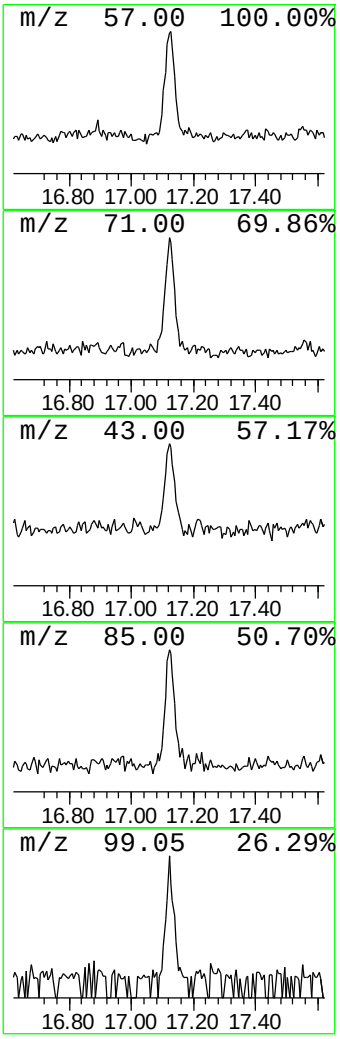
Peak Number 8 Tridecane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.12	2.39 ng	104875	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 3-methyl-	198	C14H30	006418-41-3	64
2	2-methyloctacosane	408	C29H60	1000376-72-8	64
3	2-Bromotetradecane	276	C14H29Br	074036-95-6	64
4	Heneicosane	296	C21H44	000629-94-7	64
5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	64





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...	2.20	4.7	ng	229652	1	6.89	977820	20.0
2-Pentanone, 4-hy...	5.12	3.0	ng	146700	1	6.89	977820	20.0
unknown6.66	6.66	80.8	ng	3948060	1	6.89	977820	20.0
Hexadecanoic acid...	12.81	2.4	ng	105295	5	14.05	863515	20.0
Butyl myristate	13.52	2.0	ng	86672	5	14.05	863515	20.0
Octadecane	16.52	3.0	ng	132303	6	15.54	878679	20.0
Tridecane, 3-methyl-	17.12	2.4	ng	104875	6	15.54	878679	20.0