LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF073116\
Data File : BF089472.D
Acq On : 31 Jul 2016 15:49
Operator : UM/SJ
Sample : H4257-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-COMP-2

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-BF072716.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	1.655	5	6	47	rVB	1307473	3188860	100.00%	20.240%
2	4.593	259	263	273	rBV	287554	590730	18.52%	3.749%
3	5.061	302	304	320	rBV	989069	1276221	40.02%	8.100%
4	6.159	397	400	402	rBV	1158483	1390697	43.61%	8.827%
5	6.262	407	409	411	rBV	1399429	1427819	44.78%	9.063%
6	6.490	427	429	440	rBV	214630	245974	7.71%	1.561%
7	6.650	440	443	445	rBV	878044	1042417	32.69%	6.616%
8	7.062	477	479	490	rBV	550523	841754	26.40%	5.343%
9	7.782	539	542	553	rBV	233653	332819	10.44%	2.112%
10	8.856	634	636	639	rBV	1443986	1459021	45.75%	9.261%
11	9.256	669	671	674	rBV	227497	206096	6.46%	1.308%
12	9.519	692	694	696	rBV	454016	393298	12.33%	2.496%
13	10.308	761	763	773	rVV	864107	915167	28.70%	5.809%
14	10.445	773	775	779	rVB	30597	34068	1.07%	0.216%
15	10.993	820	823	834	rBV	336817	369435	11.59%	2.345%
16	11.554	869	872	879	rBV2	33380	52614	1.65%	0.334%
17	12.422	945	948	950	rBV	25199	33886	1.06%	0.215%
18	12.571	959	961	964	rBV	978928	1045654	32.79%	6.637%
19	13.485	1038	1041	1049	rBV2	73359	113977	3.57%	0.723%
20	13.611	1049	1052	1059	rVV2	200469	260707	8.18%	1.655%
21	14.114	1093	1096	1102	rBV	58093	83302	2.61%	0.529%
22	14.605	1137	1139	1144	rVB	21500	53061	1.66%	0.337%
23	14.708	1144	1148	1156	rBV2	49486	100139	3.14%	0.636%
24	14.937	1166	1168	1177	rVB	186065	227362	7.13%	1.443%
25	16.537	1305	1308	1313	rVB2	12990	31957	1.00%	0.203%
26	17.314	1372	1376	1380	rBV2	16473	37927	1.19%	0.241%

Sum of corrected areas: 15754962

LSC Report - Integrated Chromatogram

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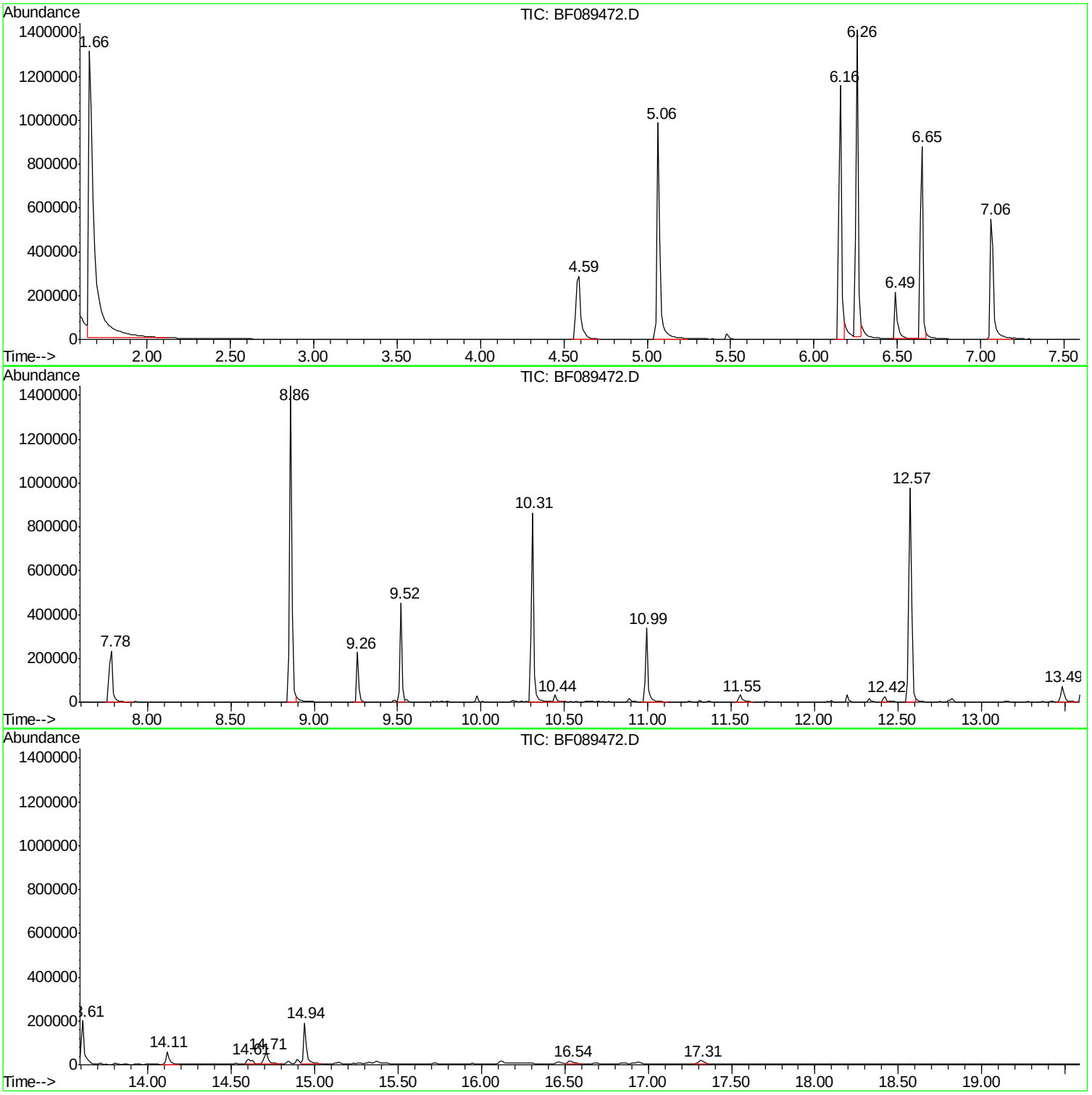
Data File : BF089472.D
Acq On : 31 Jul 2016 15:49
Operator : UM/SJ
Sample : H4257-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-COMP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.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\BF073116\
Data File : BF089472.D
Acq On : 31 Jul 2016 15:49
Operator : UM/SJ
Sample : H4257-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-COMP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

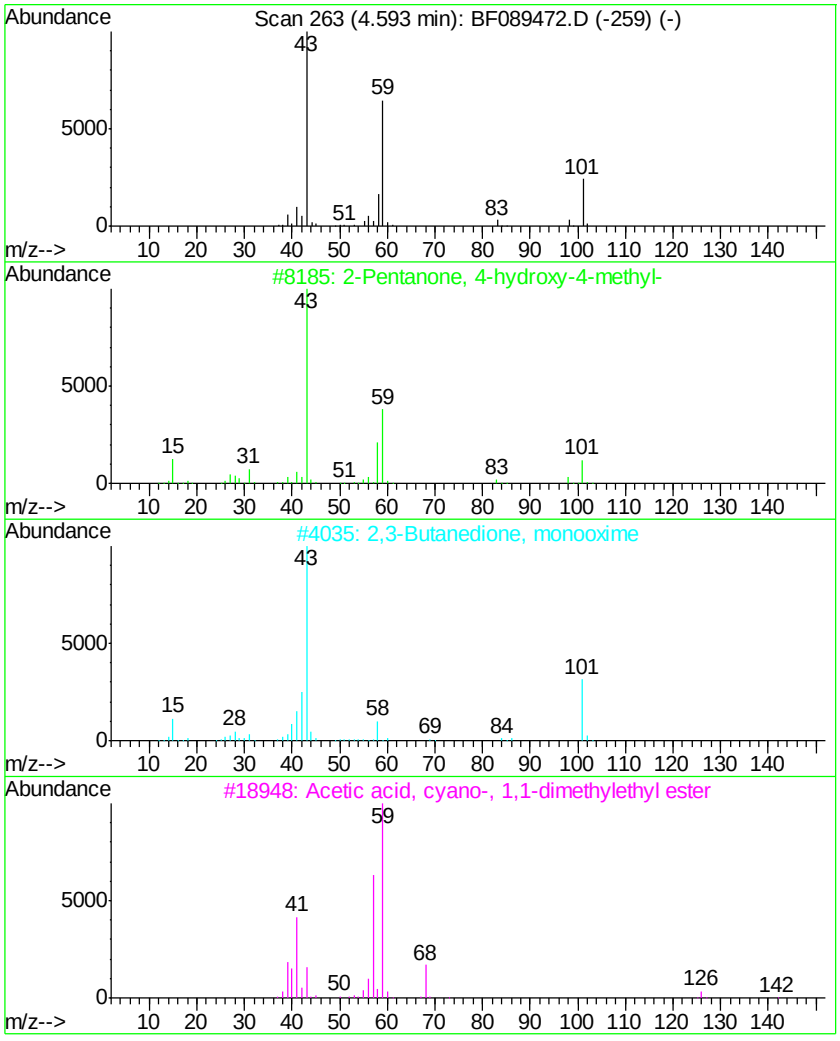
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

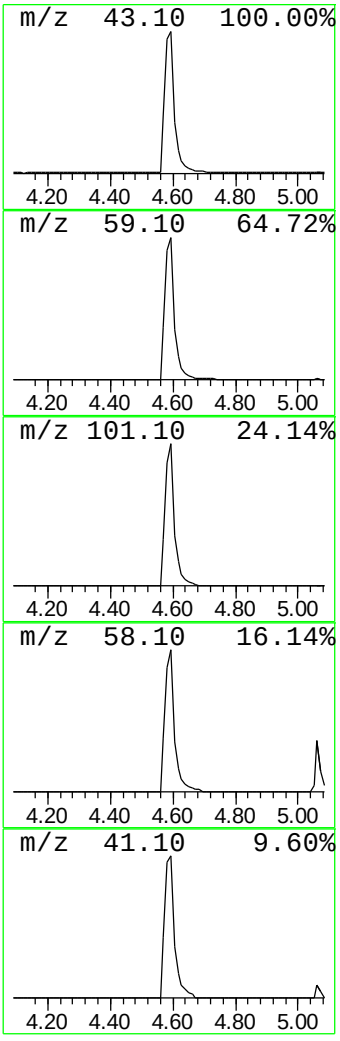
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.59	48.03 ng	590730	1,4-Dichlorobenzene-d4	6.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Acetone	58	C3H6O	000067-64-1	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF073116\
Data File : BF089472.D
Acq On : 31 Jul 2016 15:49
Operator : UM/SJ
Sample : H4257-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-COMP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

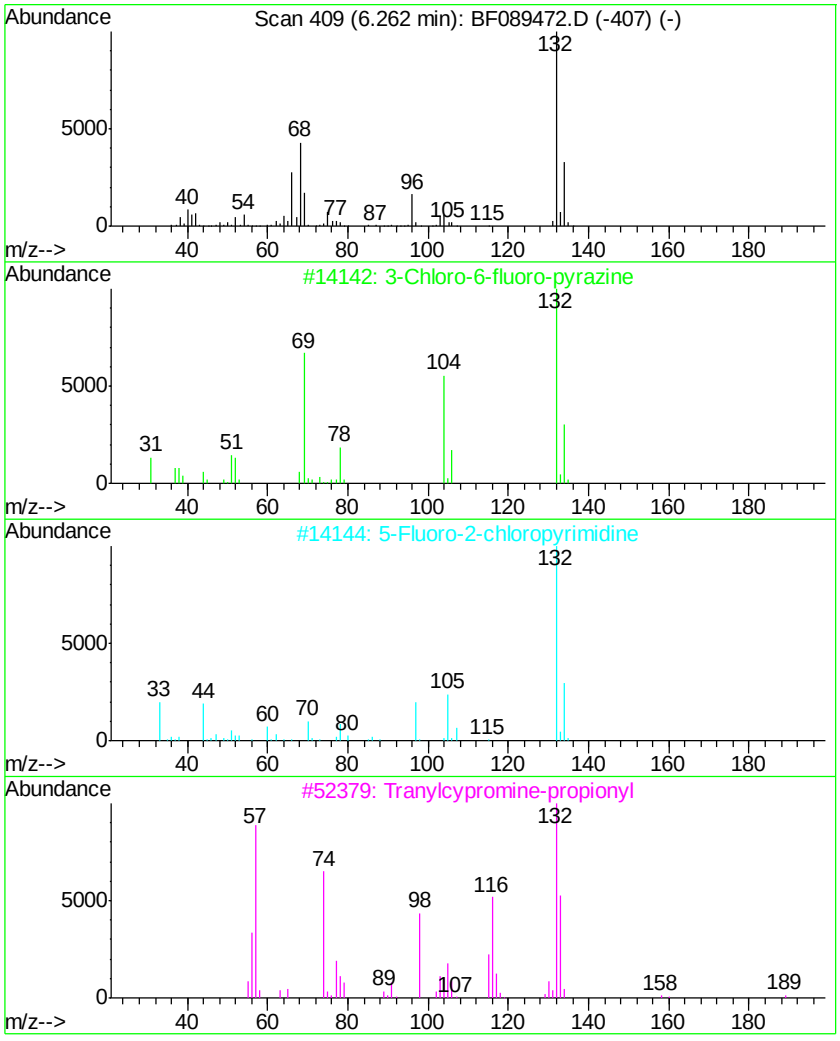
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

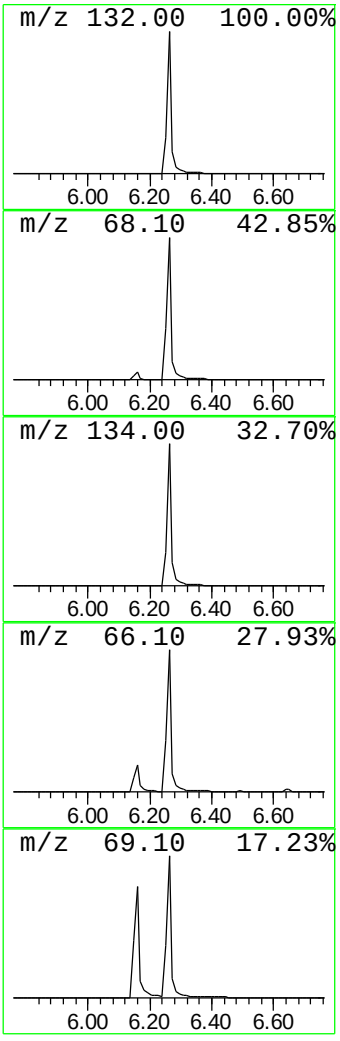
****

Peak Number 3 unknown6.26 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	116.10 ng	1427820	1,4-Dichlorobenzene-d4	6.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF073116\
Data File : BF089472.D
Acq On : 31 Jul 2016 15:49
Operator : UM/SJ
Sample : H4257-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-COMP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

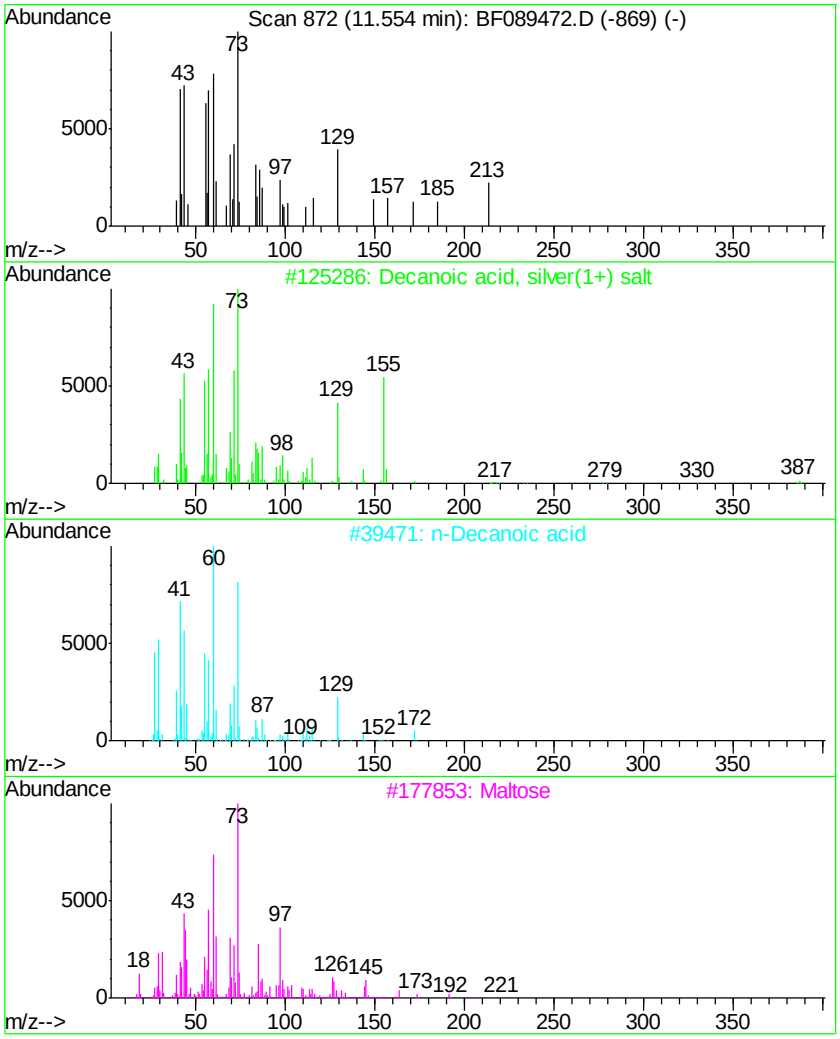
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

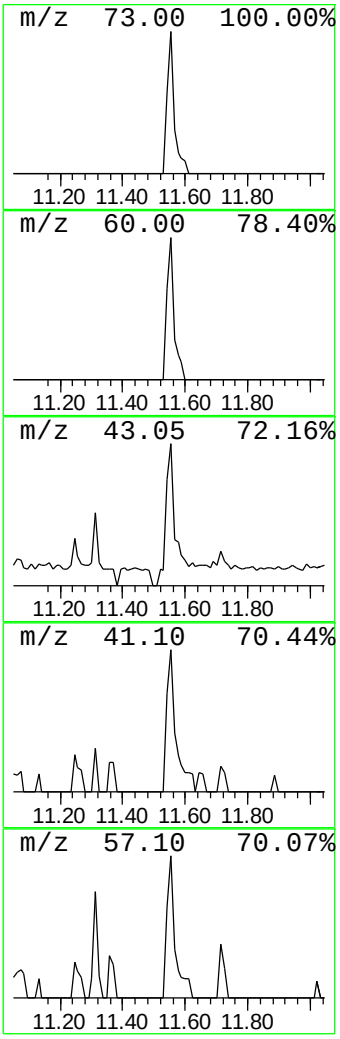
****

Peak Number 5 Decanoic acid, silver(1+) salt Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.55	2.85 ng	52614	Phenanthrene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	59
2	n-Decanoic acid	172	C10H20O2	000334-48-5	50
3	Maltose	342	C12H22O11	000069-79-4	35
4	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	22
5	Sedoheptulosan	192	C7H12O6	000469-90-9	22





Data Path : Z:\HPCHEM1\BNA F\DATA\BF073116\
Data File : BF089472.D
Acq On : 31 Jul 2016 15:49
Operator : UM/SJ
Sample : H4257-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-COMP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

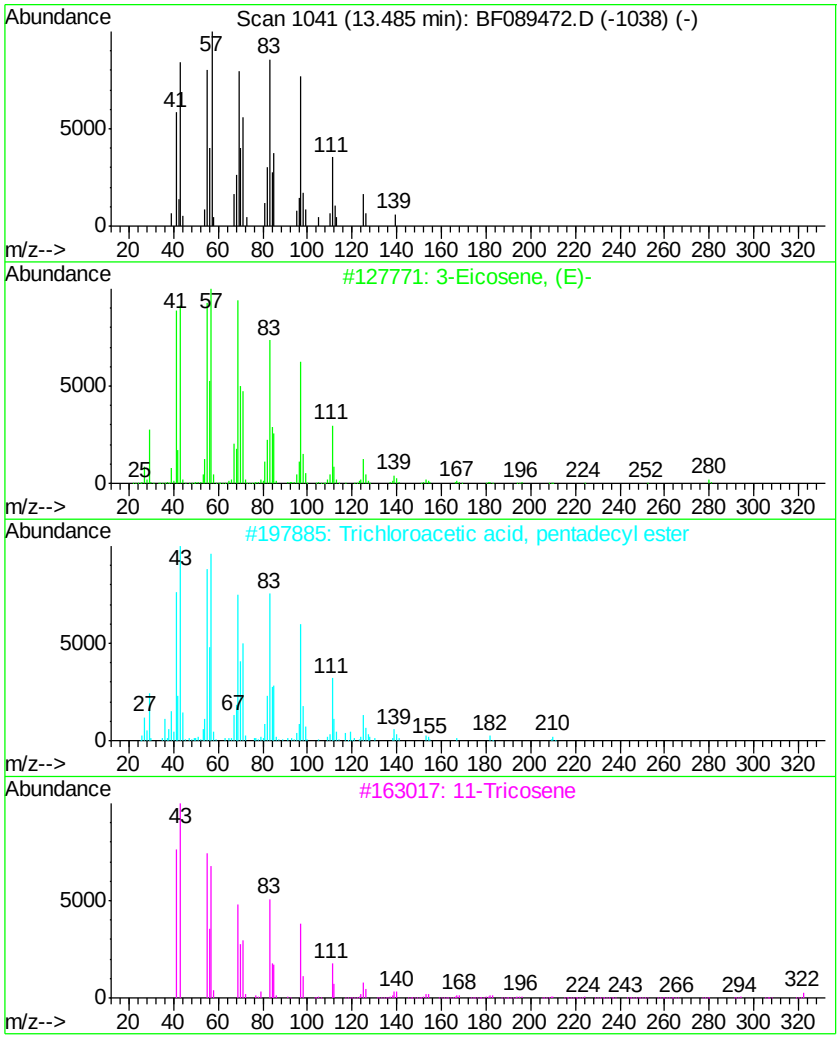
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

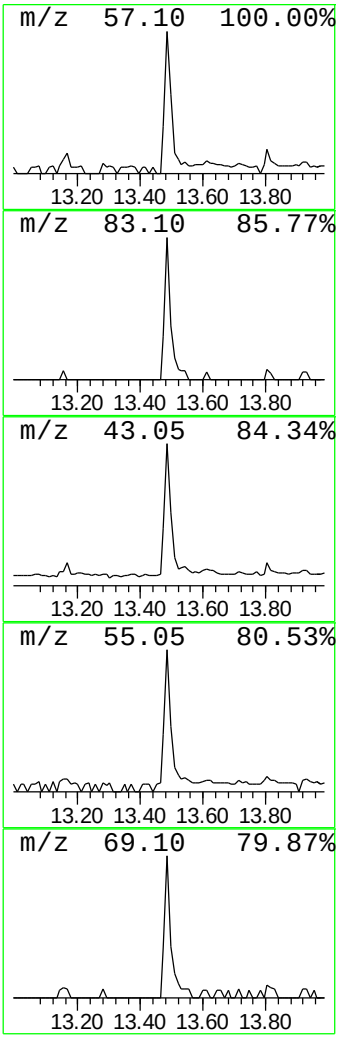
****

Peak Number 6 3-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	8.74 ng	113977	Chrysene-d12	13.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
3	11-Tricosene	322	C23H46	052078-56-5	87
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	74
5	1-Docosene	308	C22H44	001599-67-3	70





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF073116\
Data File : BF089472.D
Acq On : 31 Jul 2016 15:49
Operator : UM/SJ
Sample : H4257-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-COMP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

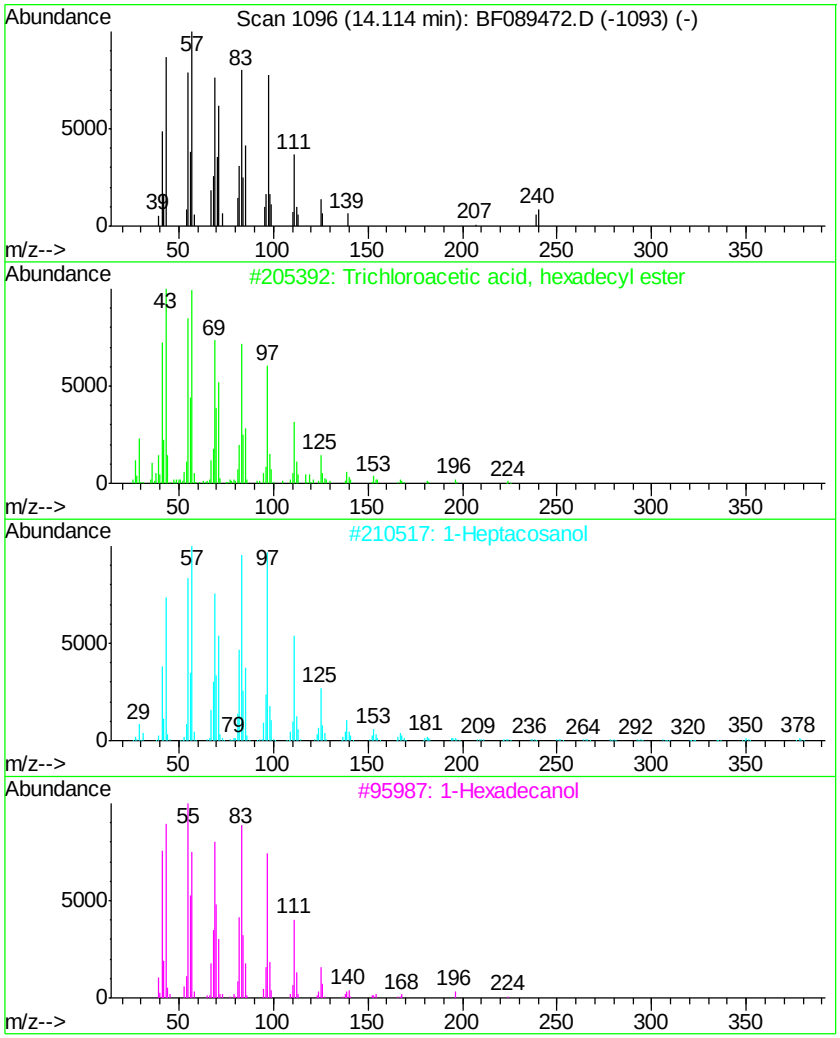
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

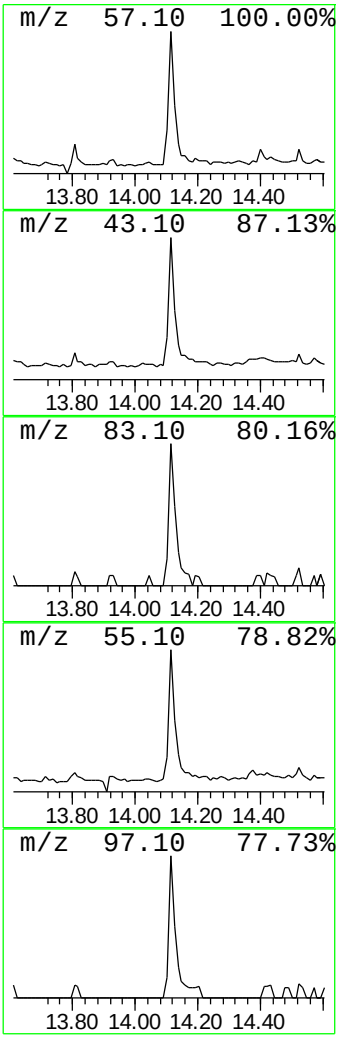
****

Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.11	6.39 ng	83302	Chrysene-d12	13.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
2	1-Heptacosanol	396	C27H56O	002004-39-9	90
3	1-Hexadecanol	242	C16H34O	036653-82-4	87
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	87
5	Behenic alcohol	326	C22H46O	000661-19-8	87





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Acq On : 31 Jul 2016 15:49
Operator : UM/SJ
Sample : H4257-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-COMP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

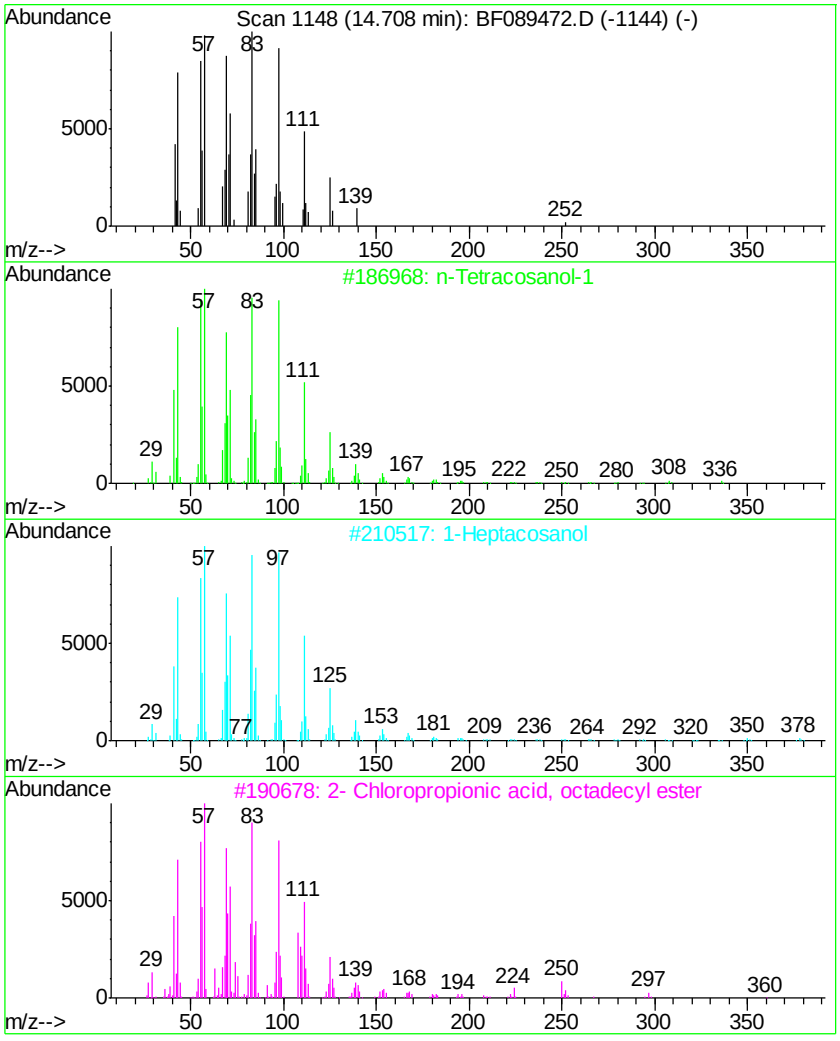
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

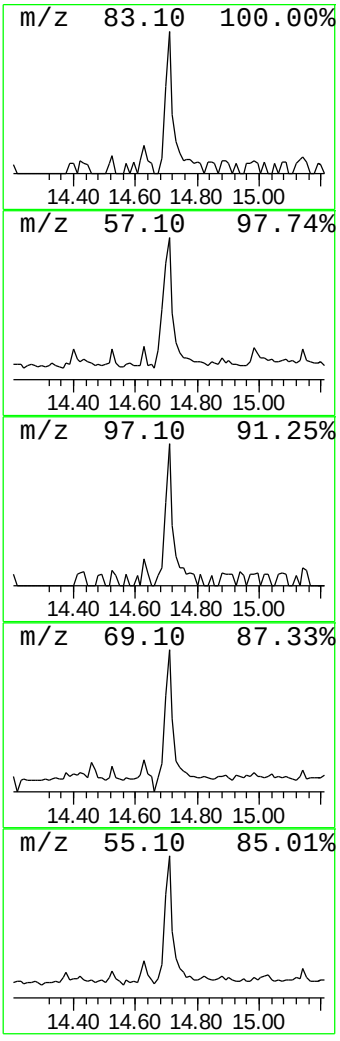
****

Peak Number 8 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	8.81 ng	100139	Perylene-d12	14.94

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	95
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
4	Octacosanol	410	C28H58O	000557-61-9	93
5	Behenic alcohol	326	C22H46O	000661-19-8	93





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-COMP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

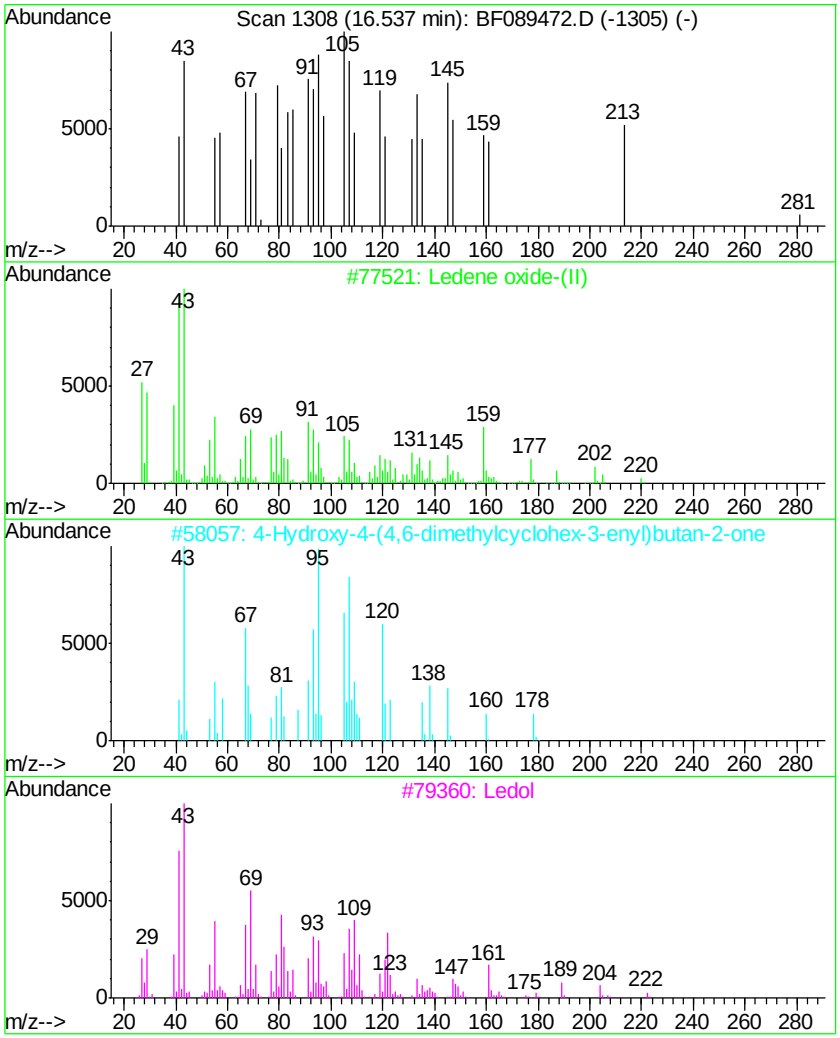
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

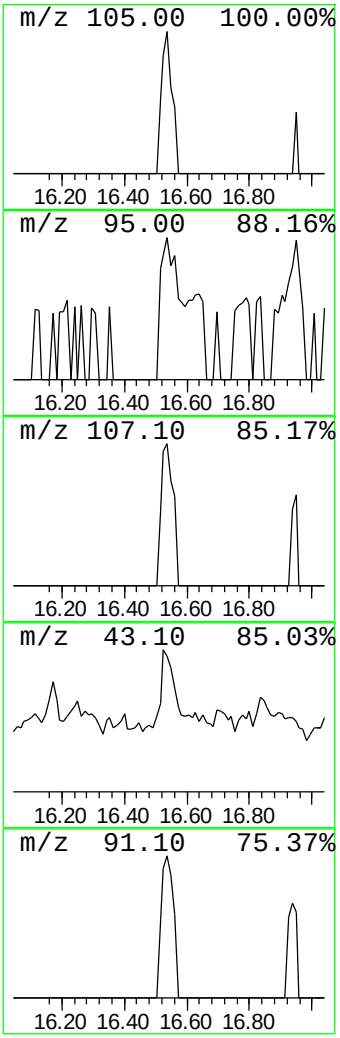
****

Peak Number 9 unknown16.54 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.54	2.81 ng	31957	Perylene-d12	14.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ledene oxide-(II)	220	C15H24O	1000159-36-7	35
2	4-Hydroxy-4-(4,6-dimethylcyclohe...	196	C12H20O2	002316-79-2	22
3	Ledol	222	C15H26O	000577-27-5	17
4	10,12-Tricosadiynoic acid, methy...	360	C24H40O2	1000333-59-4	16
5	Cyclohexane, 1,5-diethenyl-2,3-d...	164	C12H20	068779-14-6	14





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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

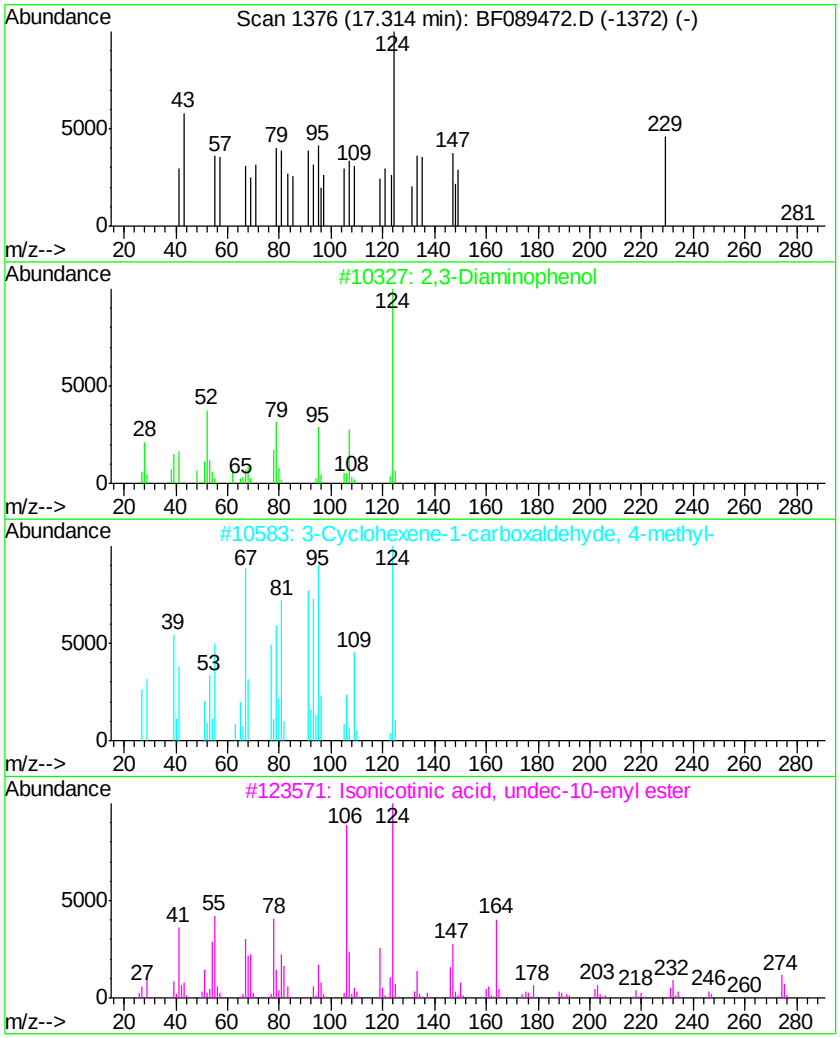
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

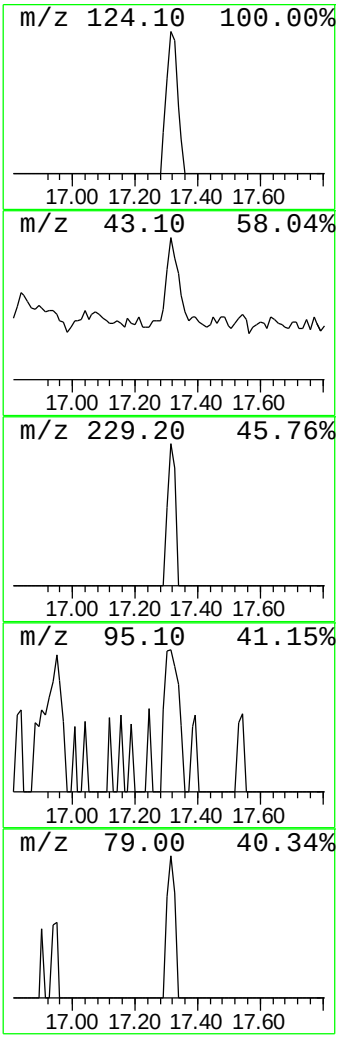
****

Peak Number 10 unknown17.31 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.31	3.34 ng	37927	Perylene-d12	14.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Diaminophenol	124	C6H8N2O	059649-56-8	30
2	3-Cyclohexene-1-carboxaldehyde, ...	124	C8H12O	007560-64-7	27
3	Isonicotinic acid, undec-10-envl...	275	C17H25NO2	1000299-88-6	27
4	5-Chlorovaleric acid, 2,6-dimeth...	284	C16H25ClO2	1000292-48-0	23
5	9-Oxabicyclo[3.3.1]nonan-2-ol, a...	184	C10H16O3	010555-34-7	16





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073116\
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Operator : UM/SJ
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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
2-Pentanone, 4-hy...	4.59	48.0	ng	590730	1	6.49	245974	20.0
unknown6.26	6.26	116.1	ng	1427820	1	6.49	245974	20.0
Decanoic acid, si...	11.55	2.9	ng	52614	4	10.99	369435	20.0
3-Eicosene, (E)-	13.49	8.7	ng	113977	5	13.61	260707	20.0
Trichloroacetic a...	14.11	6.4	ng	83302	5	13.61	260707	20.0
n-Tetracosanol-1	14.71	8.8	ng	100139	6	14.94	227362	20.0
unknown16.54	16.54	2.8	ng	31957	6	14.94	227362	20.0
unknown17.31	17.31	3.3	ng	37927	6	14.94	227362	20.0