LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
Data File : BF098935.D
Acq On : 29 Sep 2017 4:32
Operator : SJ/JU
Sample : I5485-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WALDWICK-SWITCH

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-BF092317.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	2.263	24	30	37	rVB	185343	264804	4.96%	0.930%
2	2.475	61	66	76	rVB	192582	264038	4.94%	0.927%
3	4.545	414	418	426	rBV	249949	263849	4.94%	0.927%
4	4.840	465	468	482	rBV	41060	60834	1.14%	0.214%
5	5.175	516	525	528	rBV	2824651	5341275	100.00%	18.762%
6	5.545	583	588	591	rBV	2458827	2225527	41.67%	7.818%
7	6.545	752	758	768	rBV	2349157	2603704	48.75%	9.146%
8	6.687	778	782	785	rBV	2624622	2301393	43.09%	8.084%
9	6.916	818	821	825	rVB	946967	760012	14.23%	2.670%
10	7.075	843	848	851	rBV	2831826	2430645	45.51%	8.538%
11	7.481	911	917	920	rBV	1915230	1787939	33.47%	6.281%
12	8.198	1035	1039	1043	rBV	1036276	859009	16.08%	3.017%
13	9.275	1216	1222	1225	rBV	3109345	2773659	51.93%	9.743%
14	9.663	1284	1288	1291	rBV	264392	209163	3.92%	0.735%
15	9.957	1333	1338	1345	rVB	796879	728944	13.65%	2.561%
16	10.739	1468	1471	1482	rVB	833447	734152	13.74%	2.579%
17	10.845	1486	1489	1495	rBV	177868	153901	2.88%	0.541%
18	11.445	1587	1591	1594	rBV	734497	679409	12.72%	2.387%
19	13.027	1855	1860	1863	rBV	2771998	2488334	46.59%	8.741%
20	13.910	2006	2010	2015	rBV	190983	211741	3.96%	0.744%
21	14.080	2035	2039	2043	rBV	793851	748253	14.01%	2.628%
22	15.580	2289	2294	2302	rVB	423765	577251	10.81%	2.028%

Sum of corrected areas: 28467836

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
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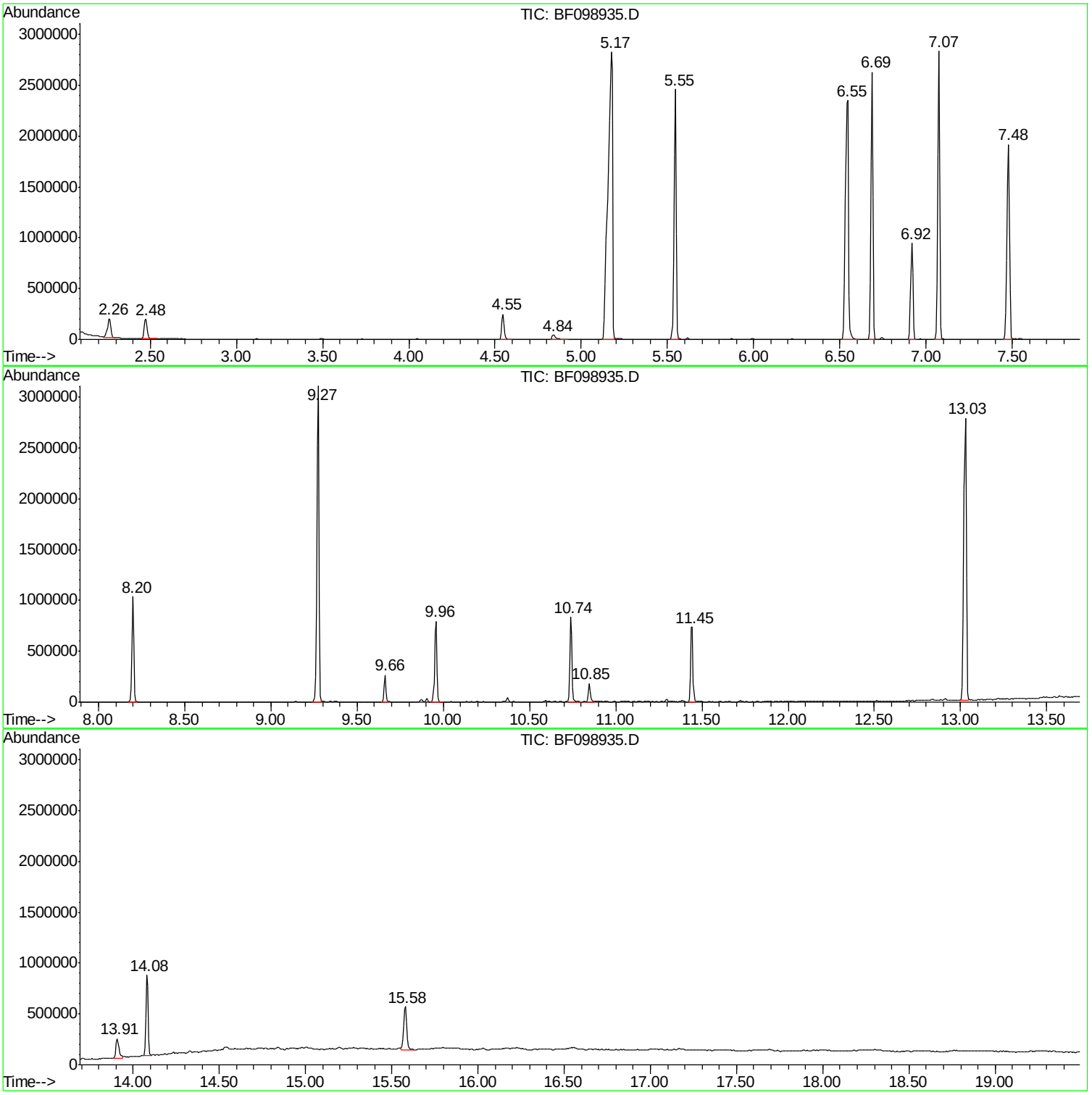
Operator : SJ/JU
Sample : I5485-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WALDWICK-SWITCH

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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\BF092817\
Data File : BF098935.D
Acq On : 29 Sep 2017 4:32
Operator : SJ/JU
Sample : I5485-01
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Instrument : BNA_F
ClientSampleId : WALDWICK-SWITCH

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

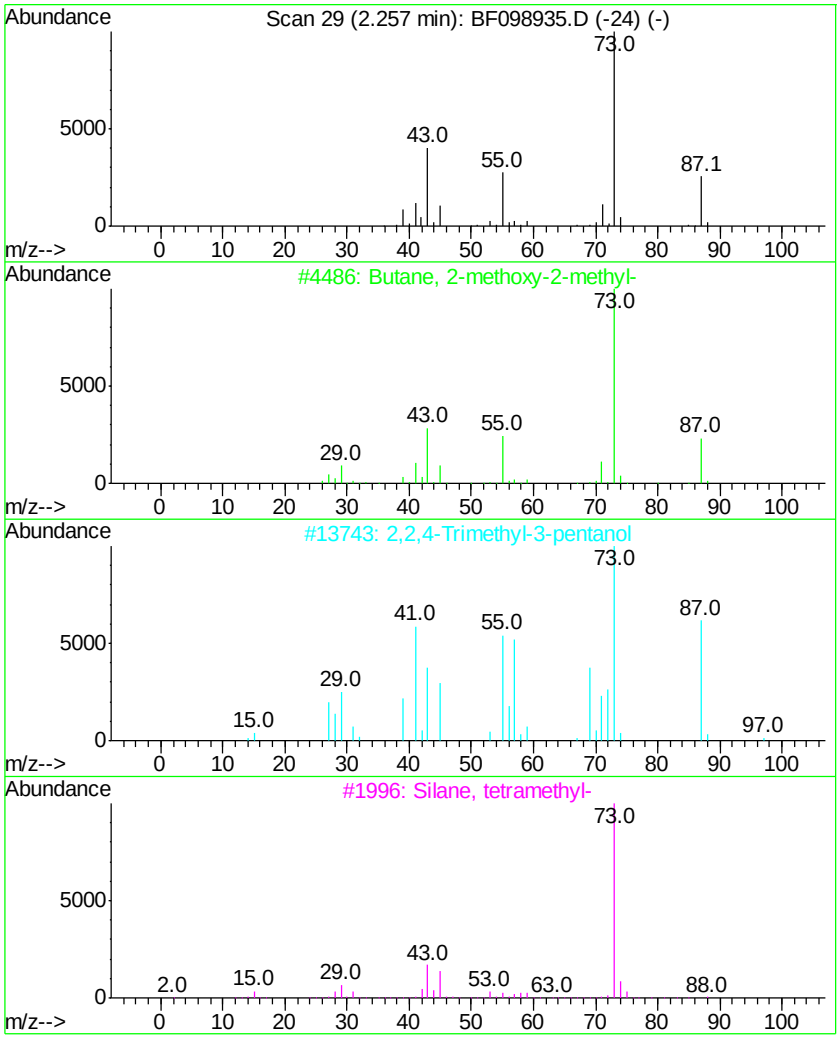
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

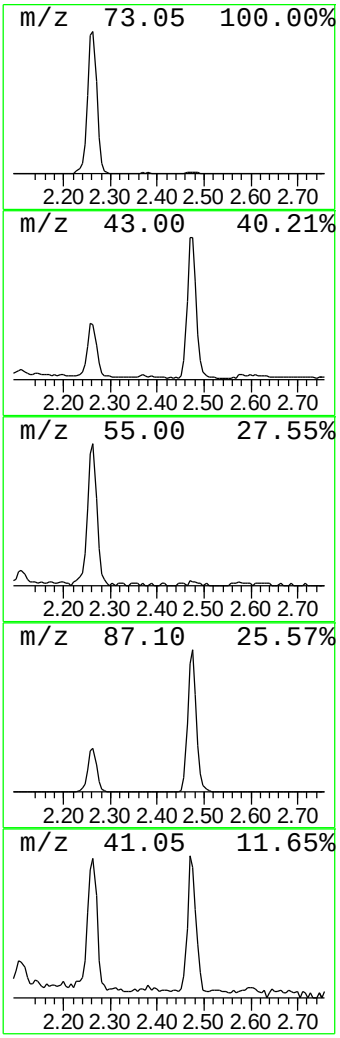
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.26	6.97 ng	264804	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	23
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17





Library Search Compound Report

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Data File : BF098935.D
Acq On : 29 Sep 2017 4:32
Operator : SJ/JU
Sample : I5485-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WALDWICK-SWITCH

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

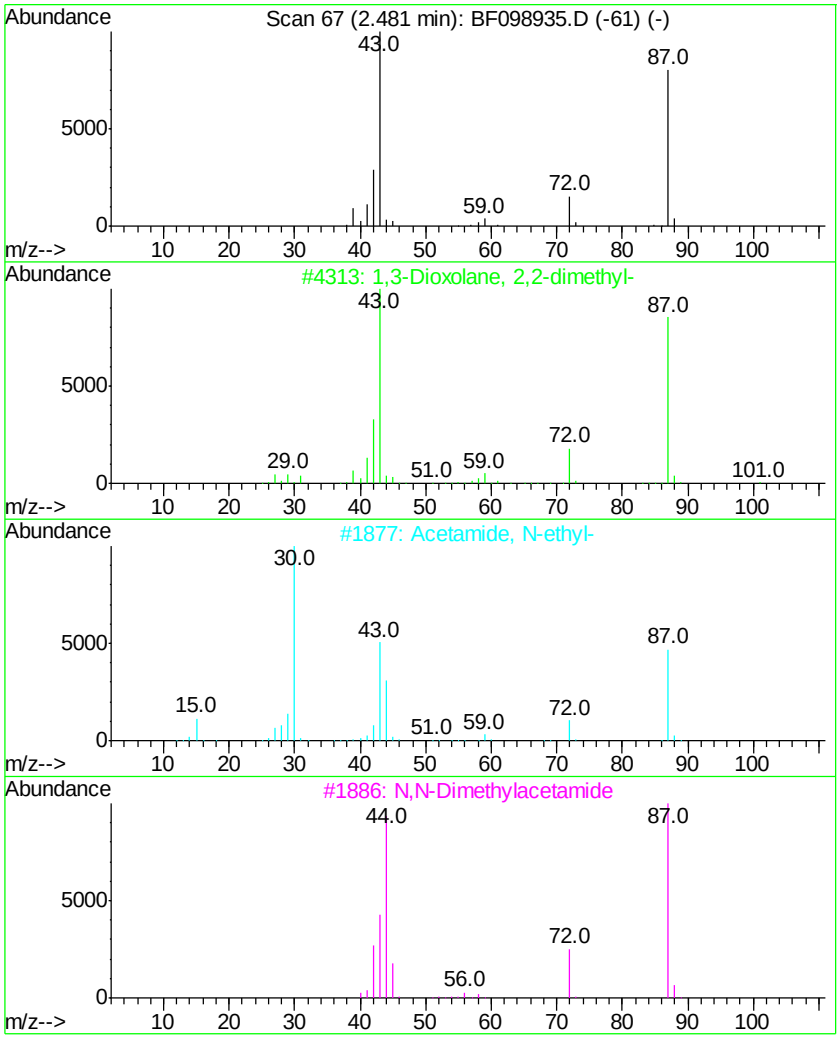
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

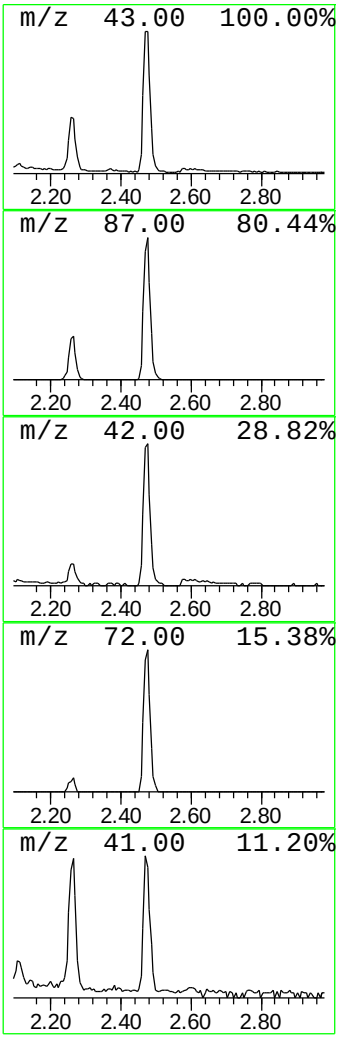
****

Peak Number 2 1,3-Dioxolane, 2,2-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.48	6.95 ng	264038	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2,2-dimethyl-	102	C5H10O2	002916-31-6	90
2	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	72
3	N,N-Dimethylacetamide	87	C4H9NO	000127-19-5	53
4	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	42
5	Ethanol, 2,2'-oxybis-, diacetate	190	C8H14O5	000628-68-2	38





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Data File : BF098935.D
Acq On : 29 Sep 2017 4:32
Operator : SJ/JU
Sample : I5485-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WALDWICK-SWITCH

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

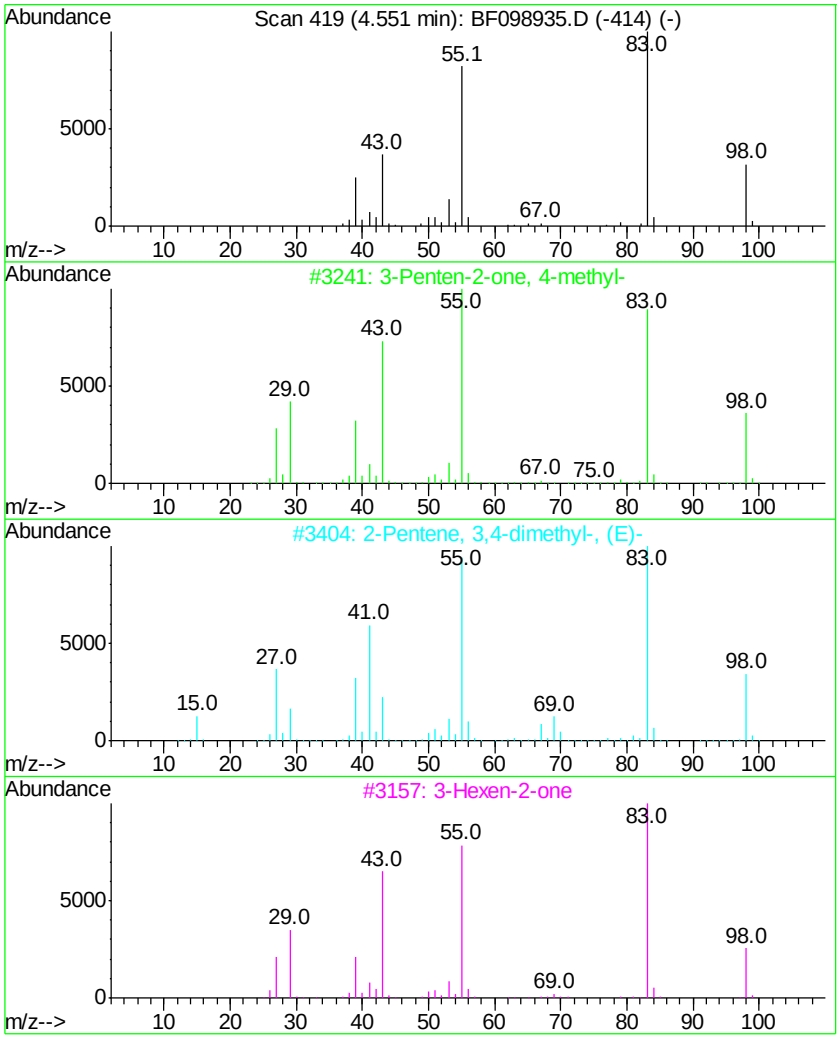
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

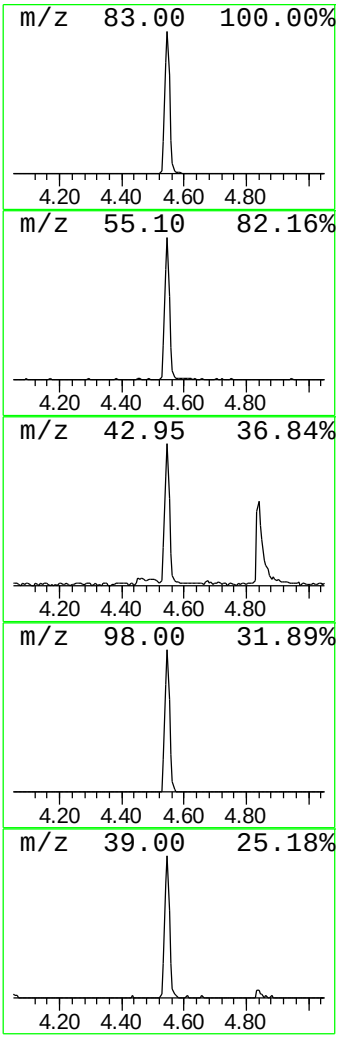
****

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	6.94 ng	263849	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3	3-Hexen-2-one	98	C6H10O	000763-93-9	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





Library Search Compound Report

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Data File : BF098935.D
Acq On : 29 Sep 2017 4:32
Operator : SJ/JU
Sample : I5485-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WALDWICK-SWITCH

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

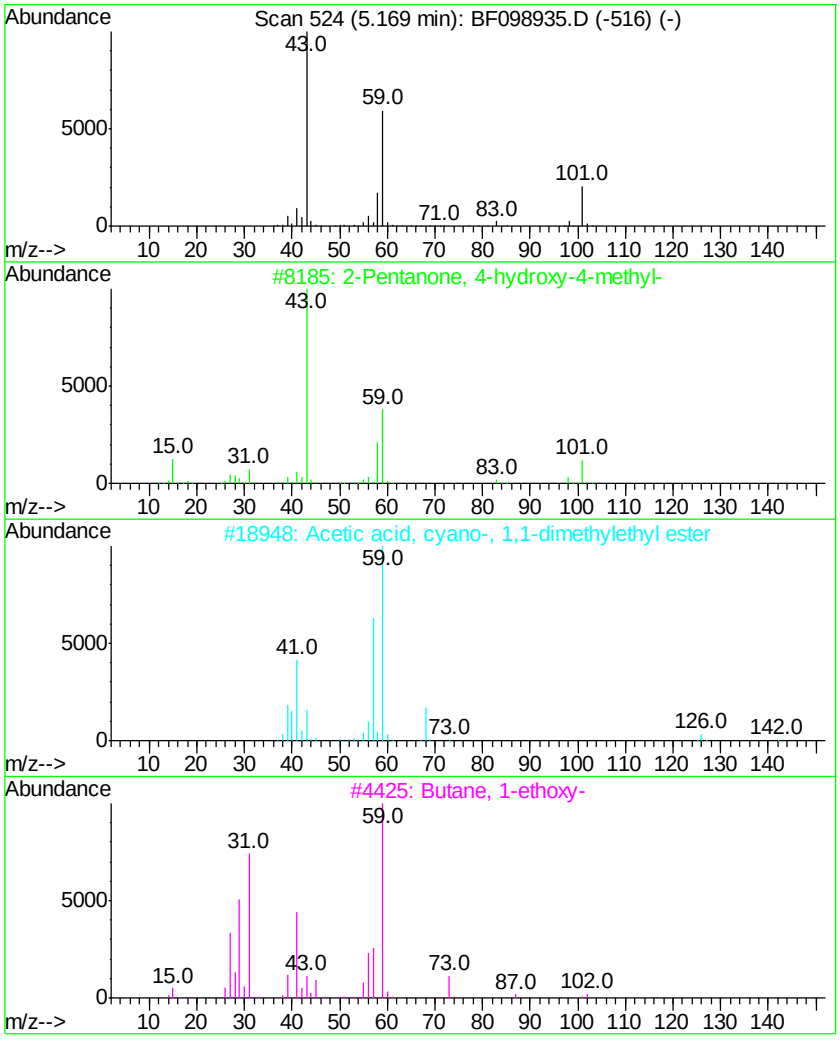
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

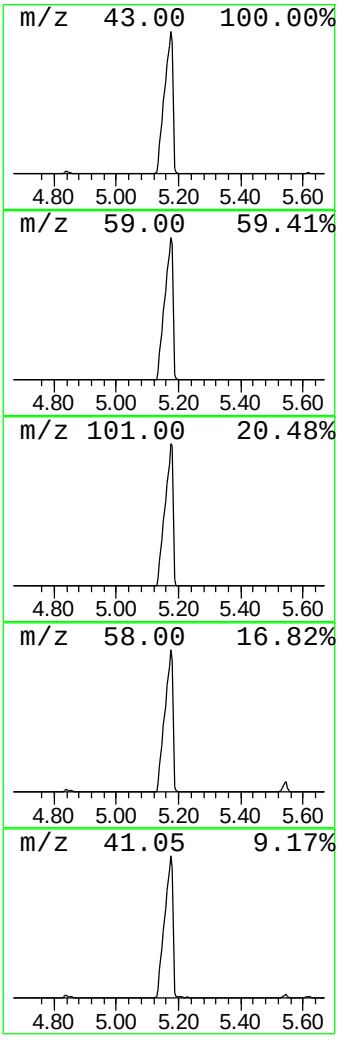
****

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	140.56 ng	5341280	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
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Sample : I5485-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WALDWICK-SWITCH

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

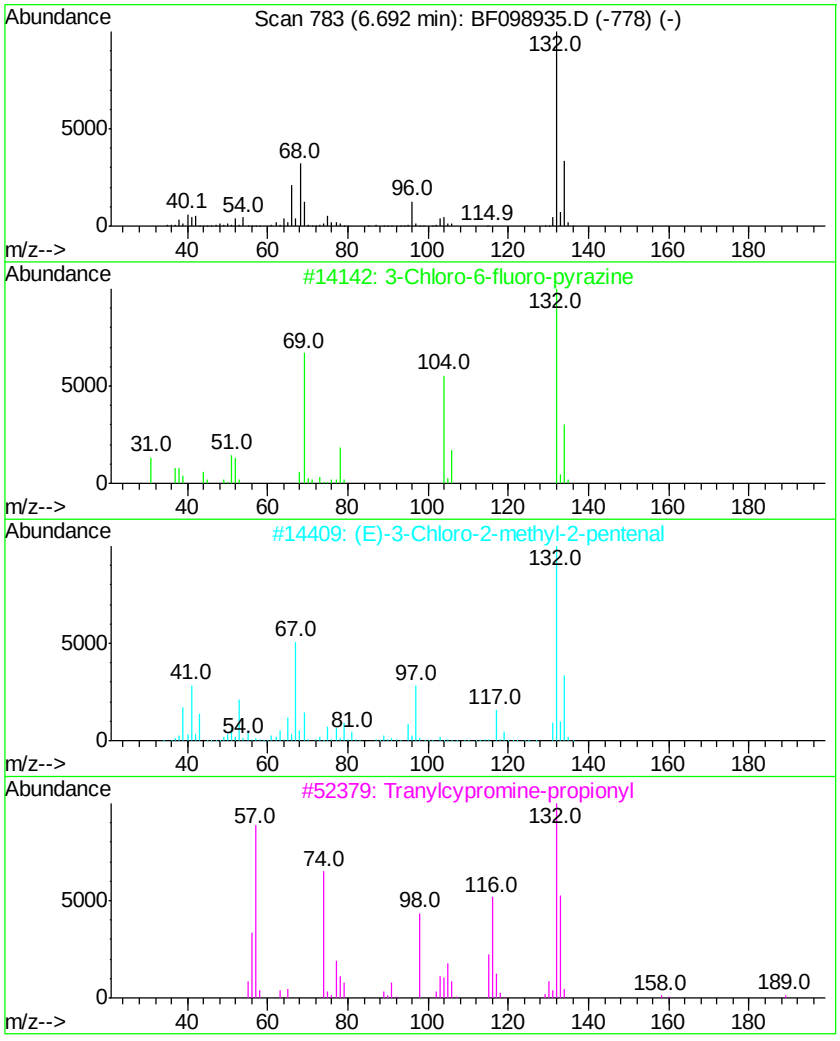
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

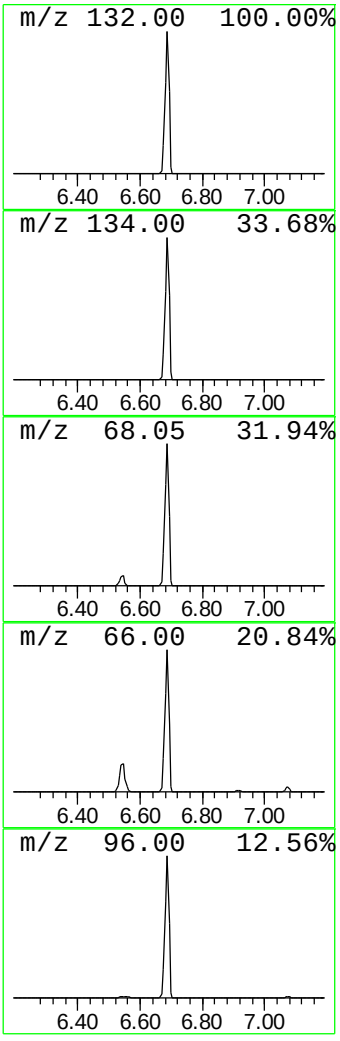
****

Peak Number 5 unknown6.69 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	60.56 ng	2301390	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : WALDWICK-SWITCH

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

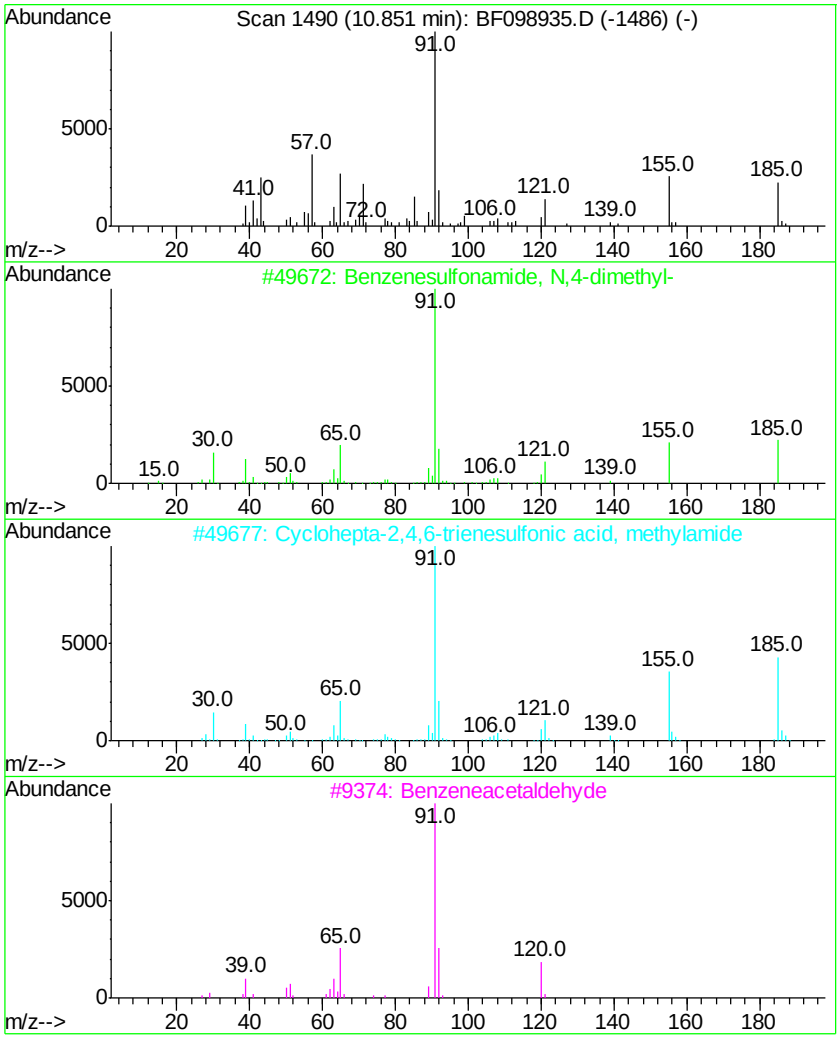
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

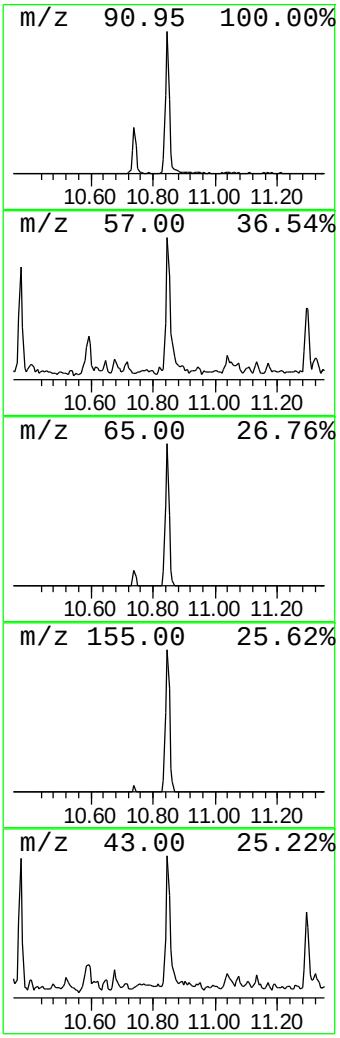
****

Peak Number 7 Benzenesulfonamide, N,4-dim... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.85	4.53 ng	153901	Phenanthrene-d10	11.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	92
2	Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	58
3	Benzeneacetaldehyde	120	C8H8O	000122-78-1	49
4	Ethyl(E/Z)-.alpha.-cyano-4-nitro...	416	C19H16N2O7S	1000287-26-8	43
5	Benzenesulfonamide, N,4-dimethyl...	214	C8H10N2O3S	000080-11-5	35





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

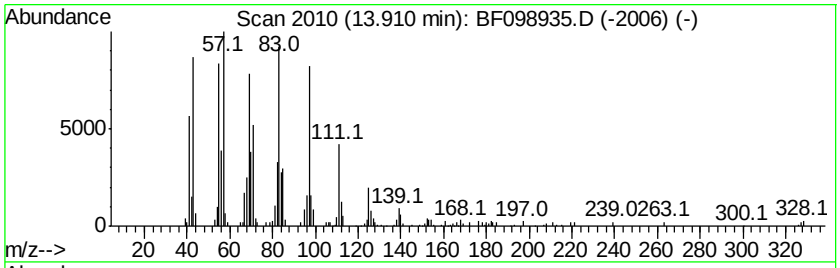
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

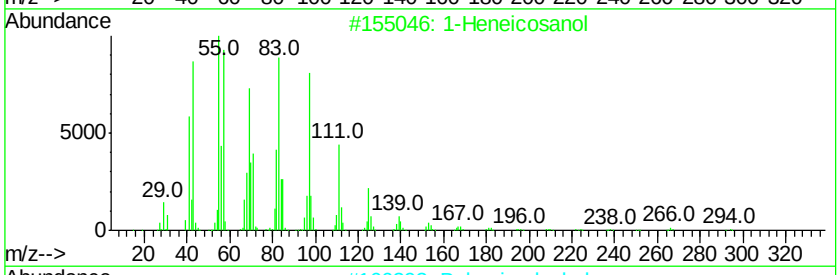
****

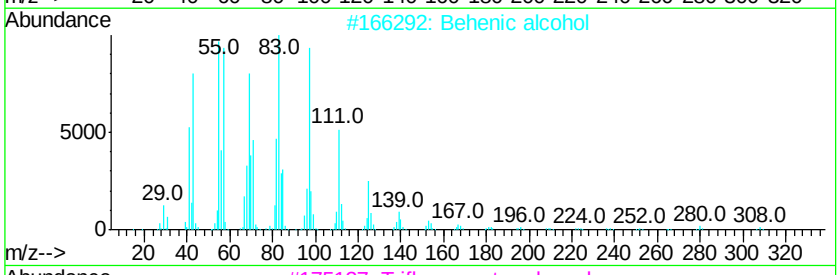
Peak Number 8 1-Heneicosanol Concentration Rank 7

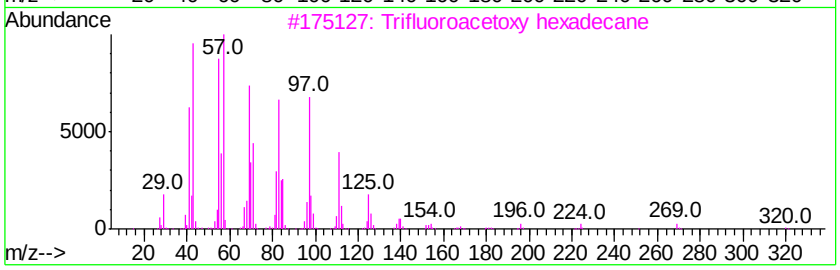
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.91	5.66 ng	211741	Chrysene-d12	14.08

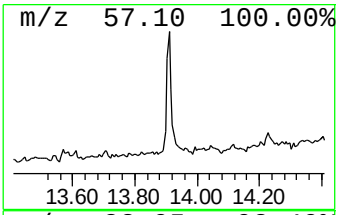
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
5	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	93

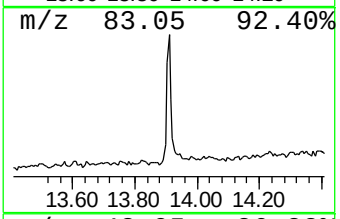


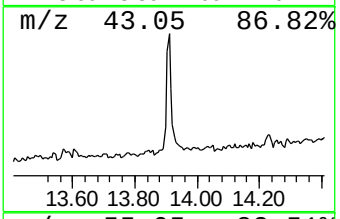


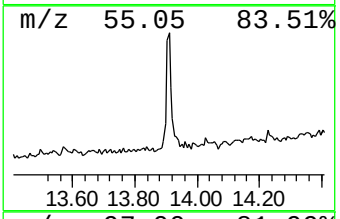


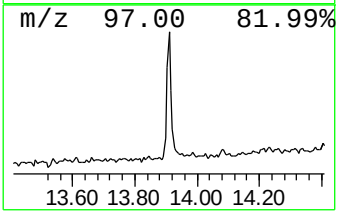












Tentatively Identified Compound (LSC) summary

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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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.26	7.0	ng	264804	1	6.92	760012	20.0
1,3-Dioxolane, 2,...	2.48	7.0	ng	264038	1	6.92	760012	20.0
3-Penten-2-one, 4...	4.55	6.9	ng	263849	1	6.92	760012	20.0
2-Pentanone, 4-hy...	5.17	140.6	ng	5341280	1	6.92	760012	20.0
unknown6.69	6.69	60.6	ng	2301390	1	6.92	760012	20.0
Benzenesulfonamid...	10.85	4.5	ng	153901	4	11.45	679409	20.0
1-Heneicosanol	13.91	5.7	ng	211741	5	14.08	748253	20.0