LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100417\
Data File : BF099080.D
Acq On : 4 Oct 2017 21:28
Operator : SJ/JU
Sample : I5616-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STONE-SP-B-COMP

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	2.175	10	15	24	rVB	150303	203329	5.82%	0.693%
2	2.999	150	155	162	rBV	48682	79290	2.27%	0.270%
3	5.098	508	512	528	rVB	398624	560238	16.05%	1.910%
4	5.493	573	579	582	rBV	2818888	2978579	85.33%	10.157%
5	6.498	744	750	753	rBV	2734703	3018353	86.47%	10.293%
6	6.634	768	773	777	rBV	2922502	3081649	88.28%	10.508%
7	6.863	808	812	816	rBV	973332	769600	22.05%	2.624%
8	7.022	834	839	842	rBV	2745932	2412105	69.10%	8.225%
9	7.428	903	908	911	rBV	1928267	1943378	55.67%	6.627%
10	8.145	1025	1030	1033	rBV	1241329	1047102	30.00%	3.571%
11	9.222	1207	1213	1216	rBV	3616534	3490644	100.00%	11.903%
12	9.610	1275	1279	1282	rBV	539645	428219	12.27%	1.460%
13	9.898	1323	1328	1332	rVB	1184739	1141076	32.69%	3.891%
14	10.322	1397	1400	1403	rVB	52577	39566	1.13%	0.135%
15	10.692	1455	1463	1466	rBV	1943722	1892237	54.21%	6.453%
16	10.792	1477	1480	1486	rBV	62194	60807	1.74%	0.207%
17	11.386	1577	1581	1585	rBV	1315760	1110022	31.80%	3.785%
18	12.974	1846	1851	1854	rBV	3095895	3038761	87.05%	10.362%
19	13.851	1997	2000	2008	rBV	155965	175162	5.02%	0.597%
20	14.027	2026	2030	2033	rBV	863610	820847	23.52%	2.799%
21	14.486	2104	2108	2114	rBV3	78138	104210	2.99%	0.355%
22	15.121	2213	2216	2220	rBV	55332	61143	1.75%	0.208%
23	15.498	2274	2280	2289	rBV	496699	630192	18.05%	2.149%
24	15.710	2312	2316	2319	rBV3	29842	39215	1.12%	0.134%
25	15.939	2351	2355	2360	rVB	30238	47298	1.35%	0.161%
26	17.539	2623	2627	2636	rVB7	17741	40568	1.16%	0.138%
27	18.362	2758	2767	2775	rBV8	37165	111927	3.21%	0.382%

Sum of corrected areas: 29325517

LSC Report - Integrated Chromatogram

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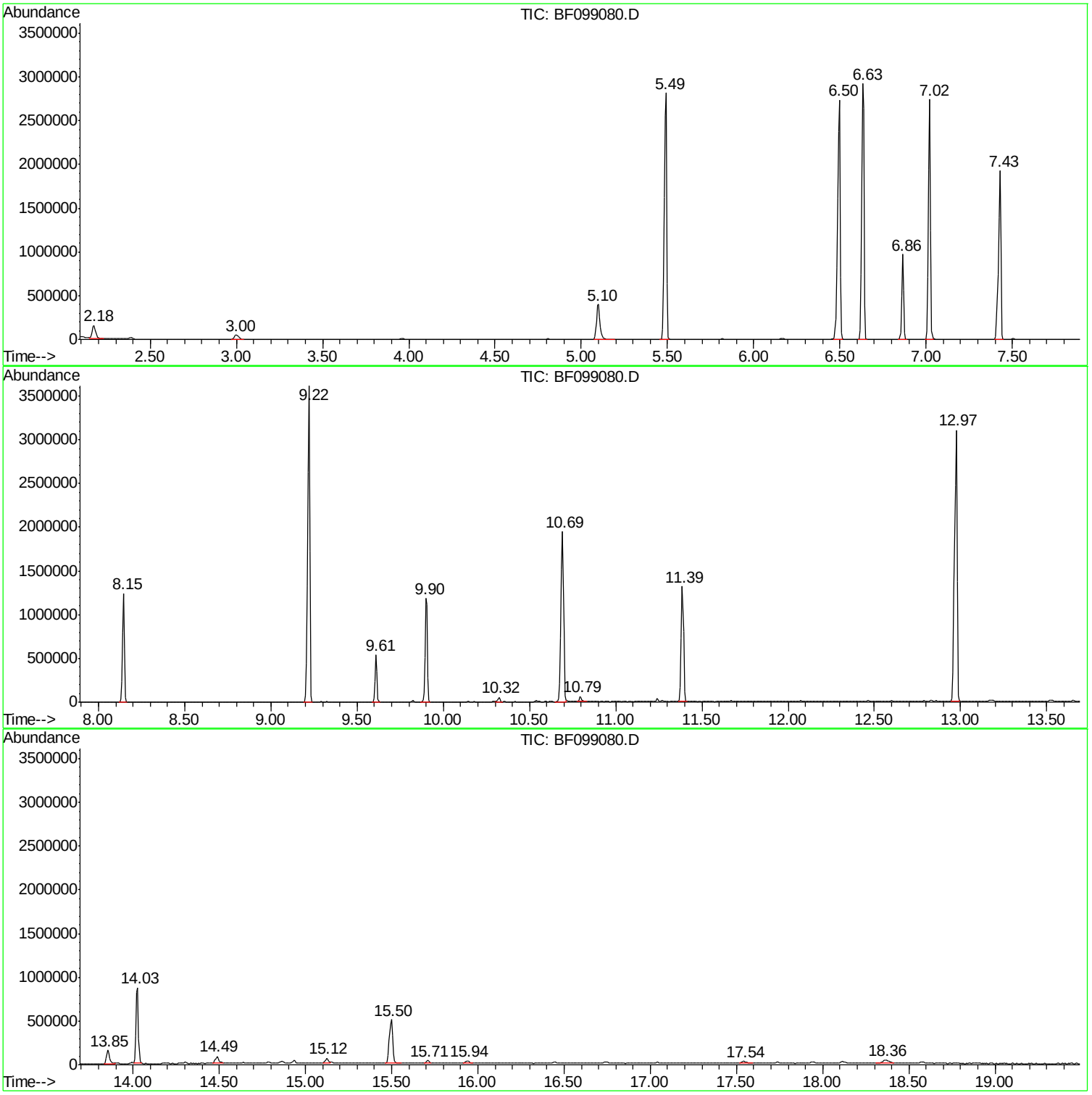
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STONE-SP-B-COMP

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\BF100417\
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Sample : I5616-05
Misc :
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Instrument : BNA_F
ClientSampleId : STONE-SP-B-COMP

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

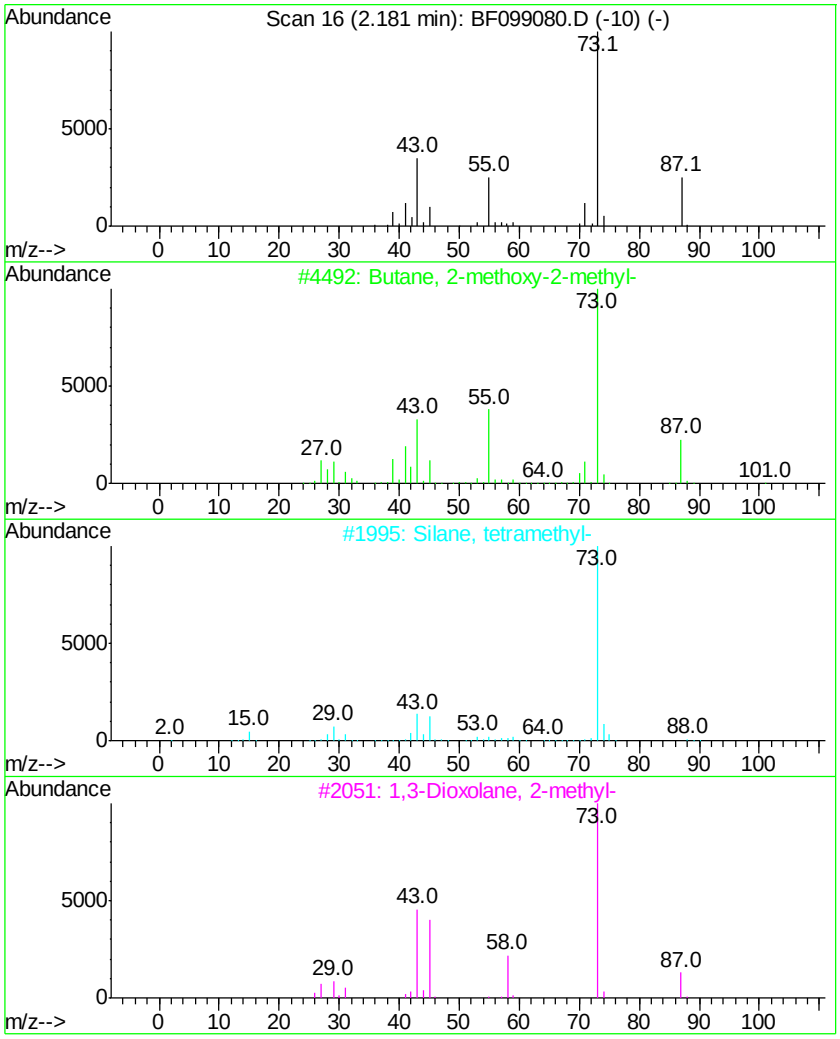
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

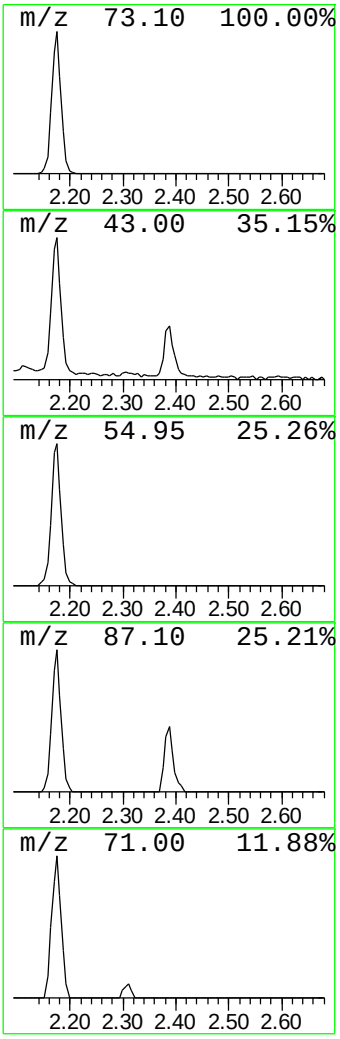
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	5.28 ng	203329	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	37
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





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Acq On : 4 Oct 2017 21:28
Operator : SJ/JU
Sample : I5616-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STONE-SP-B-COMP

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

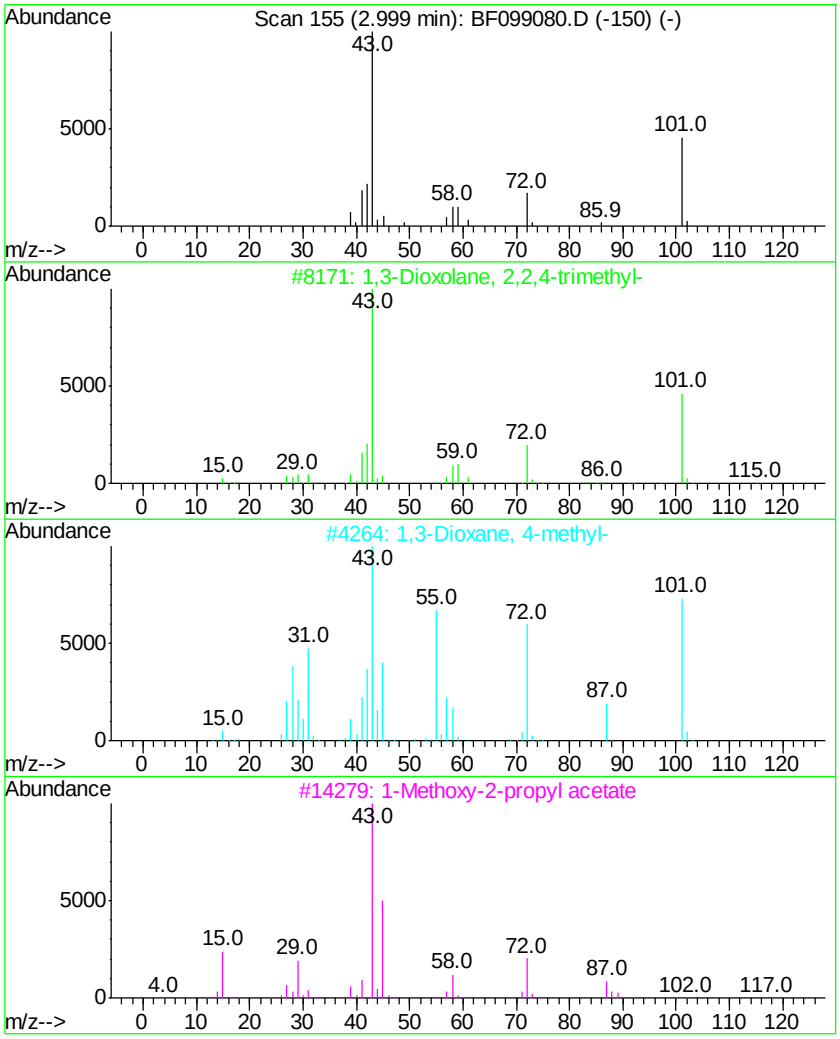
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

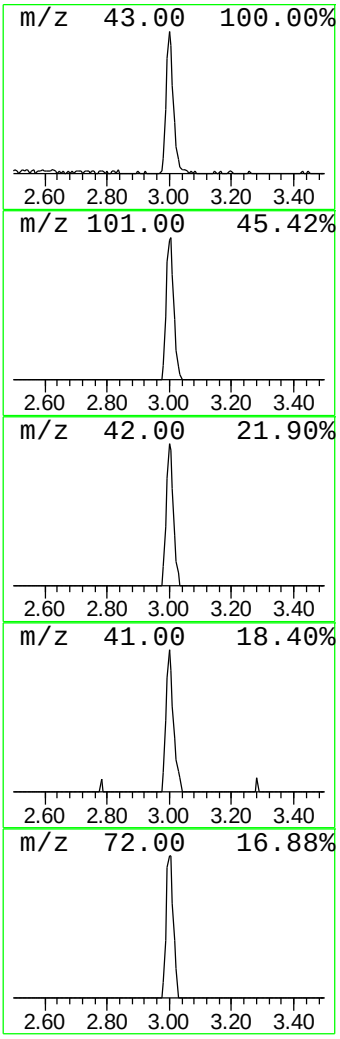
****

Peak Number 2 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.00	2.06 ng	79290	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	90
2	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	42
3	1-Methoxy-2-propyl acetate	132	C6H12O3	000108-65-6	10
4	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	9
5	Oxirane, trimethyl-	86	C5H10O	005076-19-7	9





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Acq On : 4 Oct 2017 21:28
Operator : SJ/JU
Sample : I5616-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STONE-SP-B-COMP

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

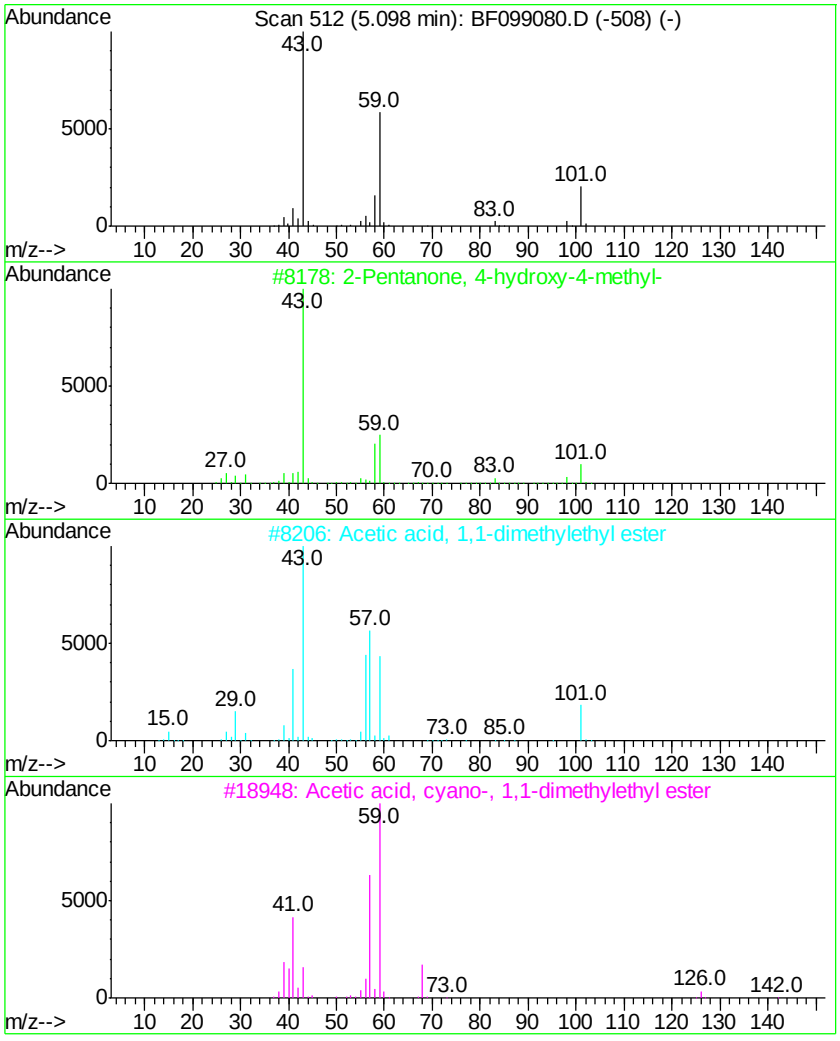
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

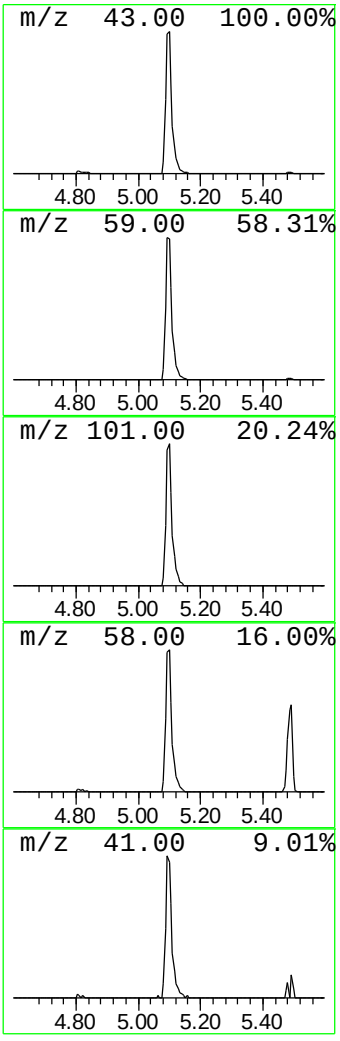
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	14.56 ng	560238	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	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100417\
Data File : BF099080.D
Acq On : 4 Oct 2017 21:28
Operator : SJ/JU
Sample : I5616-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STONE-SP-B-COMP

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

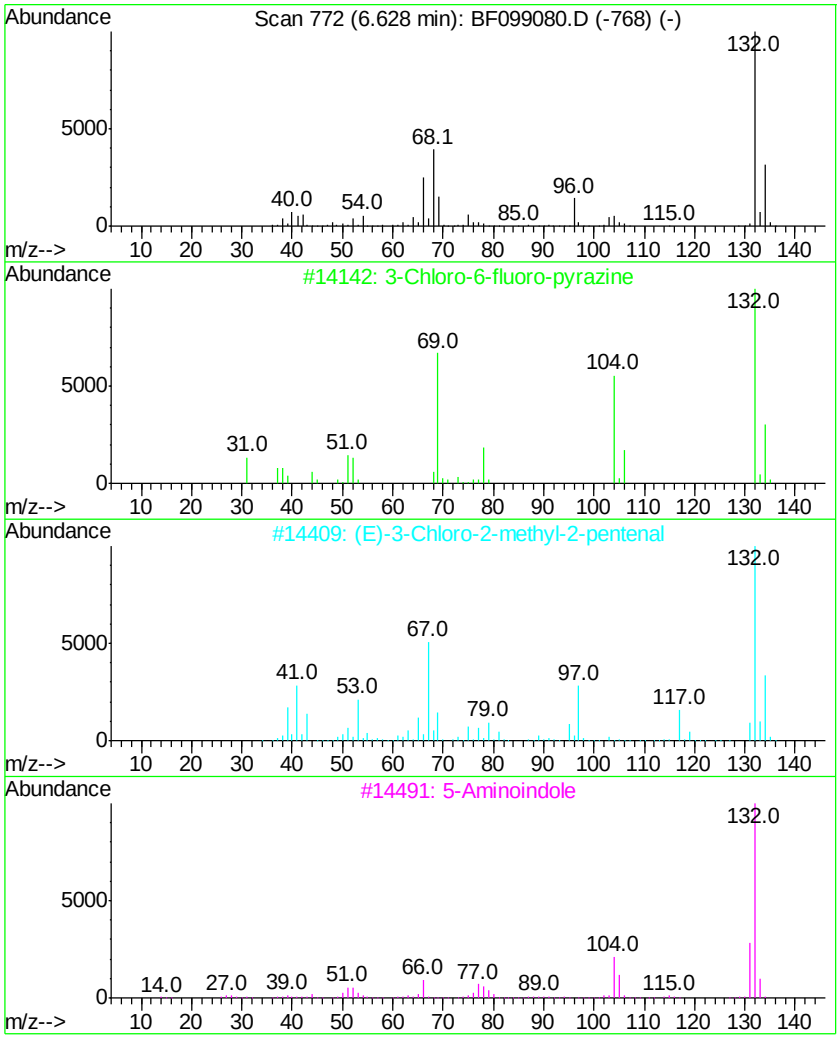
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

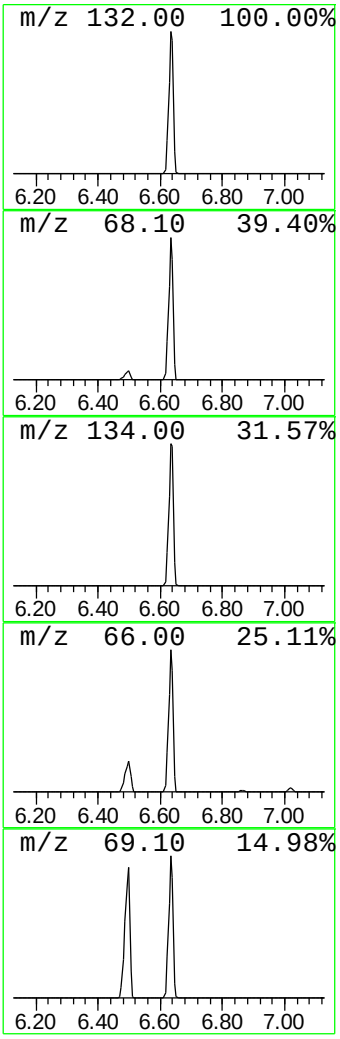
****

Peak Number 4 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	80.08 ng	3081650	1,4-Dichlorobenzene-d4	6.86

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	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100417\
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ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STONE-SP-B-COMP

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

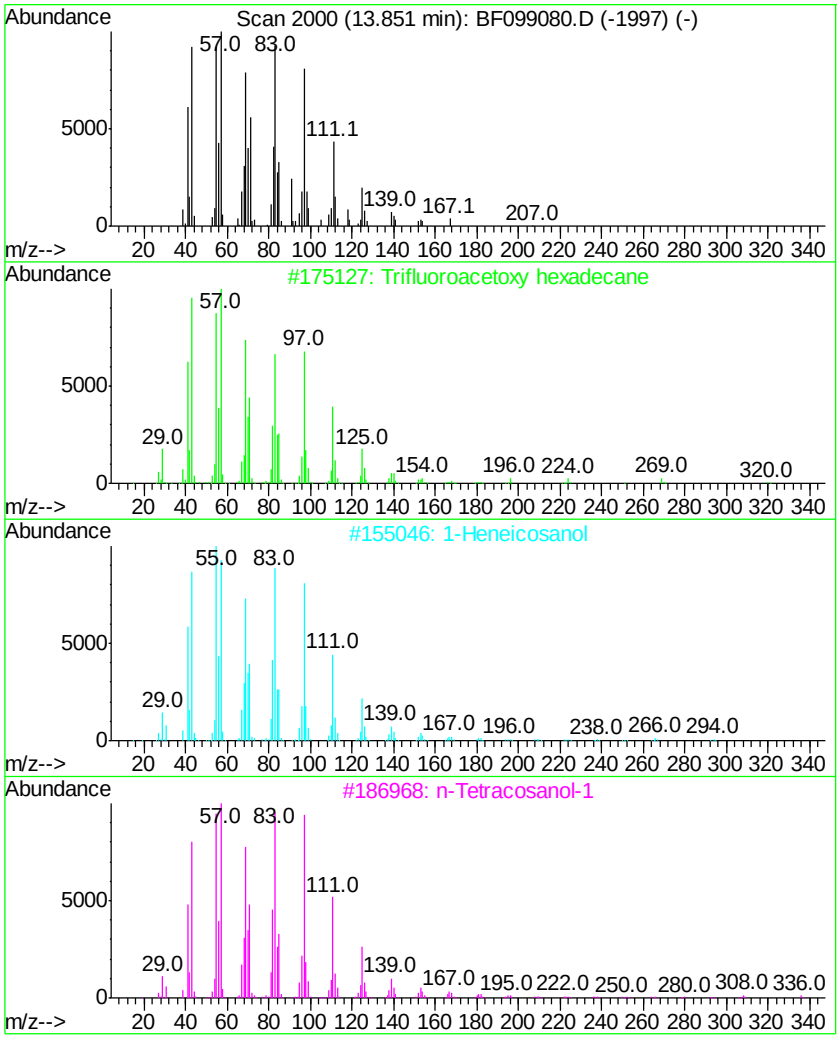
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

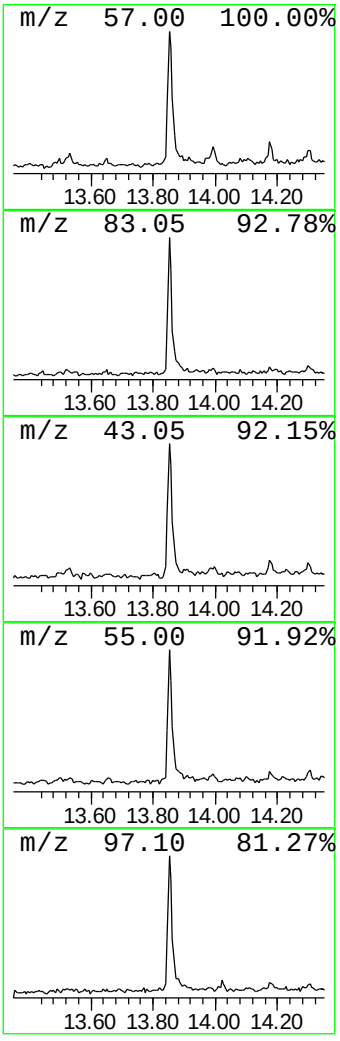
****

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	4.27 ng	175162	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	1-Heptacosanol	396	C27H56O	002004-39-9	91





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Instrument : BNA_F
ClientSampleId : STONE-SP-B-COMP

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

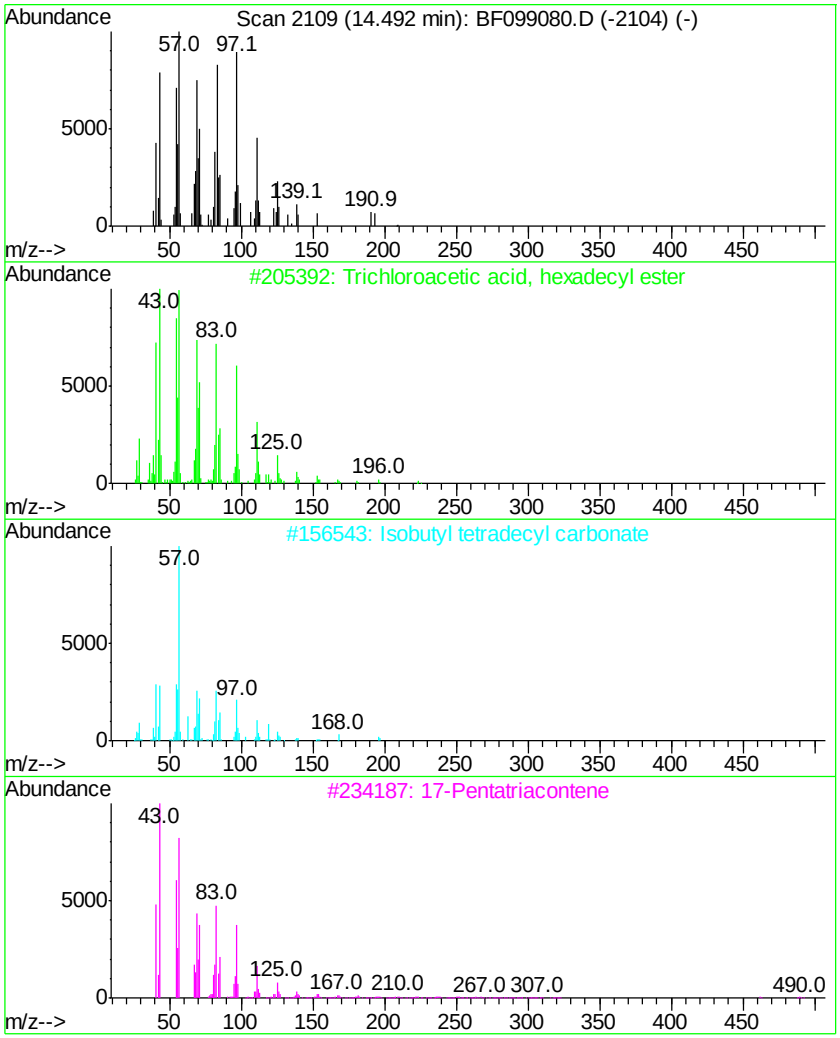
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

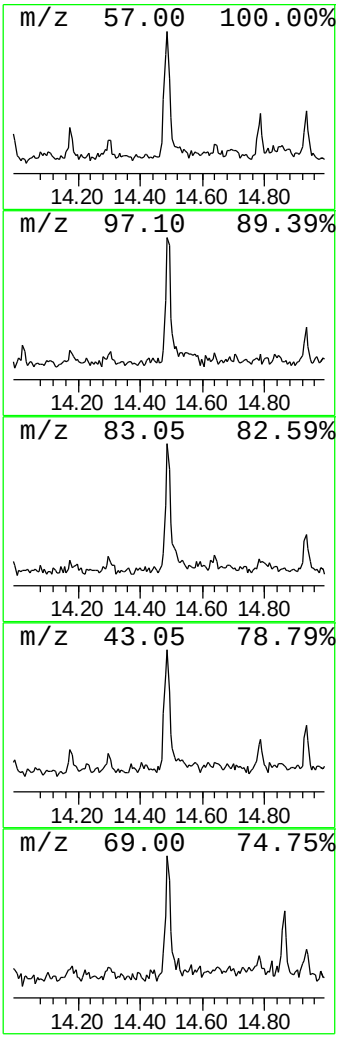
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.49	2.54 ng	104210	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2	Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	91
3	17-Pentatriacontene	491	C35H70	006971-40-0	90
4	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	87
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	87





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

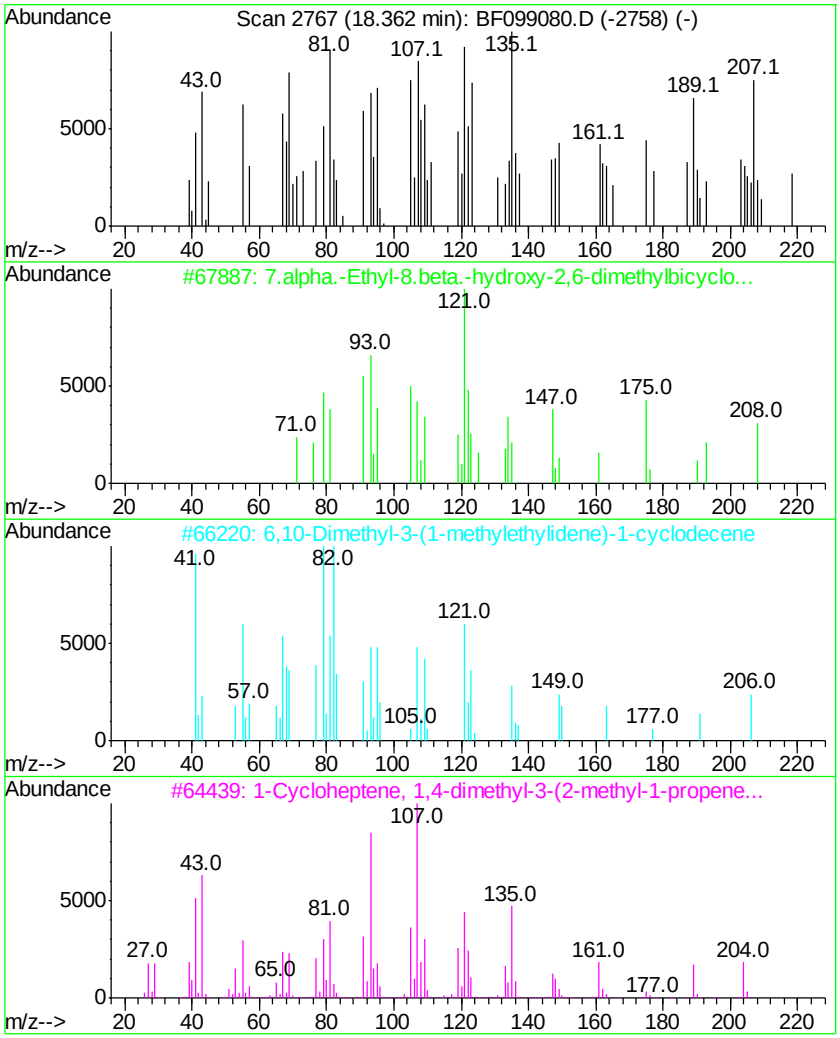
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

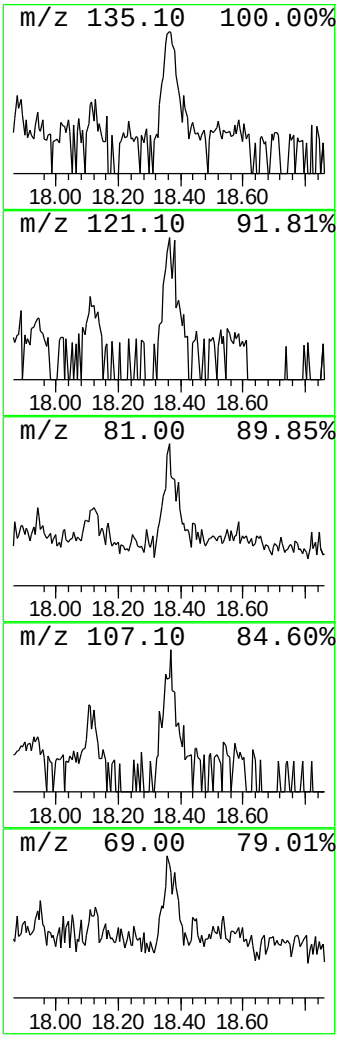
****

Peak Number 8 7.alpha.-Ethyl-8.beta.-hydr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	3.55 ng	111927	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7.alpha.-Ethyl-8.beta.-hydroxy-2...	208	C14H24O	1000077-92-4	74
2	6,10-Dimethyl-3-(1-methylethylid...	206	C15H26	069239-71-0	45
3	1-Cycloheptene, 1,4-dimethyl-3-(...	204	C15H24	1000159-38-6	42
4	2,4a,8,8-Tetramethyldecahydrocyc...	206	C15H26	074022-04-1	38
5	7.beta.-Ethyl-8.beta.-hydroxy-2,...	208	C14H24O	1000077-92-5	38





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
Butane, 2-methoxy...	2.18	5.3	ng	203329	1	6.86	769600	20.0
1,3-Dioxolane, 2,...	3.00	2.1	ng	79290	1	6.86	769600	20.0
2-Pentanone, 4-hy...	5.10	14.6	ng	560238	1	6.86	769600	20.0
unknown6.63	6.63	80.1	ng	3081650	1	6.86	769600	20.0
Trifluoroacetoxy ...	13.85	4.3	ng	175162	5	14.03	820847	20.0
Trichloroacetic a...	14.49	2.5	ng	104210	5	14.03	820847	20.0
7.alpha.-Ethyl-8....	18.36	3.5	ng	111927	6	15.50	630192	20.0