LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072417\
Data File : BF097009.D
Acq On : 25 Jul 2017 2:22
Operator : SJ/JU
Sample : I4361-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RAMP-D-1-(0-2)

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-BF071317.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	2.346	73	78	89	rVB	273292	408336	12.05%	1.354%
2	2.716	137	141	156	rBV	164490	334283	9.86%	1.109%
3	4.669	470	473	485	rVB	234824	372911	11.00%	1.237%
4	5.122	546	550	567	rBV	2983079	3300000	97.35%	10.944%
5	6.181	725	730	744	rBV	3134043	3389949	100.00%	11.242%
6	6.287	744	748	752	rBV	3064481	3131170	92.37%	10.384%
7	6.510	783	786	790	rBV	975754	867301	25.58%	2.876%
8	6.669	809	813	816	rBV	2516698	2343187	69.12%	7.771%
9	7.081	878	883	886	rBV	2152560	2108076	62.19%	6.991%
10	7.222	902	907	911	rBV	78679	94480	2.79%	0.313%
11	7.716	988	991	1000	rBV	78128	76595	2.26%	0.254%
12	7.792	1000	1004	1008	rBV	1201956	1143787	33.74%	3.793%
13	8.751	1159	1167	1174	rBV	35089	41698	1.23%	0.138%
14	8.875	1182	1188	1191	rBV	3079082	3112568	91.82%	10.322%
15	9.269	1249	1255	1259	rBV	763677	708977	20.91%	2.351%
16	9.539	1296	1301	1305	rBV2	1362747	1271414	37.51%	4.216%
17	9.963	1366	1373	1376	rBV2	43295	52855	1.56%	0.175%
18	9.998	1376	1379	1381	rVB	53042	47189	1.39%	0.156%
19	10.327	1430	1435	1438	rBV	1685936	1619837	47.78%	5.372%
20	10.463	1454	1458	1466	rBV	86869	114785	3.39%	0.381%
21	10.910	1530	1534	1537	rBV	80198	71211	2.10%	0.236%
22	11.016	1547	1552	1555	rBV	1197150	1052188	31.04%	3.489%
23	11.333	1603	1606	1612	rVB	40556	40294	1.19%	0.134%
24	11.569	1643	1646	1654	rBV2	169180	185229	5.46%	0.614%
25	12.598	1816	1821	1825	rBV	2025171	2063671	60.88%	6.844%
26	13.074	1897	1902	1906	rBV	363367	342973	10.12%	1.137%
27	13.510	1971	1976	1984	rBV	154439	207516	6.12%	0.688%
28	13.639	1994	1998	2002	rBV	785915	785282	23.17%	2.604%
29	14.139	2080	2083	2093	rVB2	29886	40918	1.21%	0.136%
30	14.992	2223	2228	2233	rBV	572797	643456	18.98%	2.134%
31	15.404	2294	2298	2302	rBV	38643	55484	1.64%	0.184%
32	15.821	2365	2369	2375	rBV3	29160	48269	1.42%	0.160%
33	16.315	2446	2453	2457	rBV3	23063	42228	1.25%	0.140%
34	16.880	2545	2549	2556	rVB5	17034	36235	1.07%	0.120%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072417\
Data File : BF097009.D
Acq On : 25 Jul 2017 2:22
Operator : SJ/JU
Sample : I4361-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RAMP-D-1-(0-2)

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-BF071317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

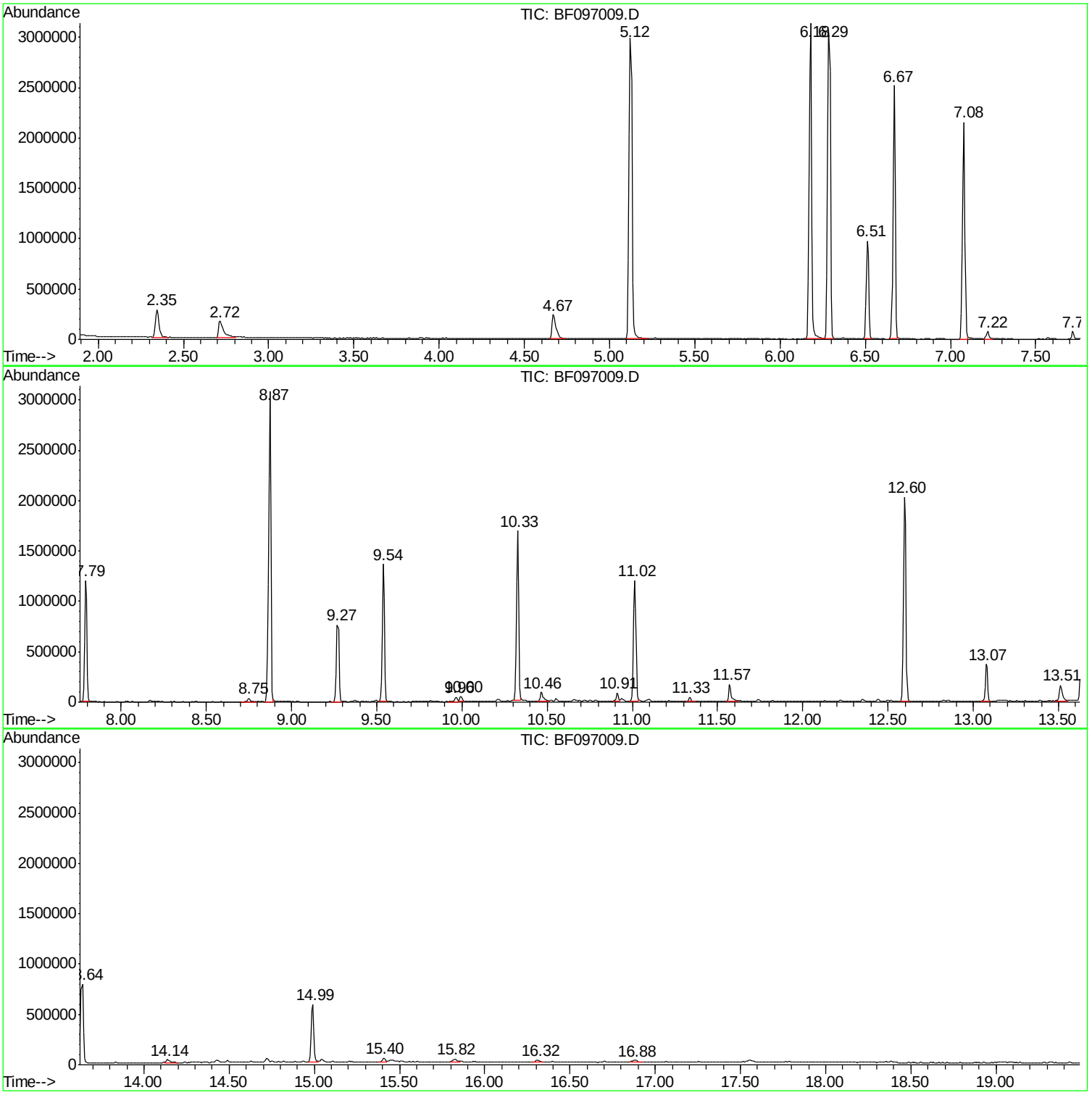
Sum of corrected areas: 30154352

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072417\
Data File : BF097009.D
Acq On : 25 Jul 2017 2:22
Operator : SJ/JU
Sample : I4361-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RAMP-D-1-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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\BF072417\
Data File : BF097009.D
Acq On : 25 Jul 2017 2:22
Operator : SJ/JU
Sample : I4361-01
Misc :
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Instrument : BNA_F
ClientSampleId : RAMP-D-1-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

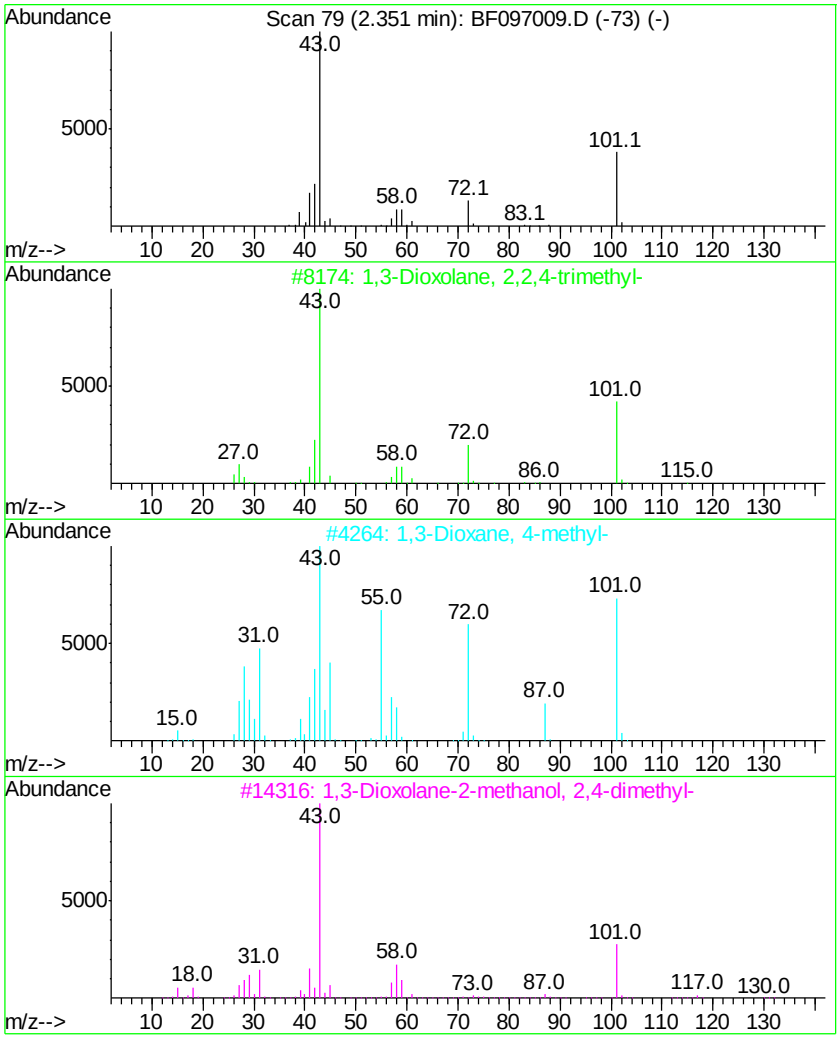
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

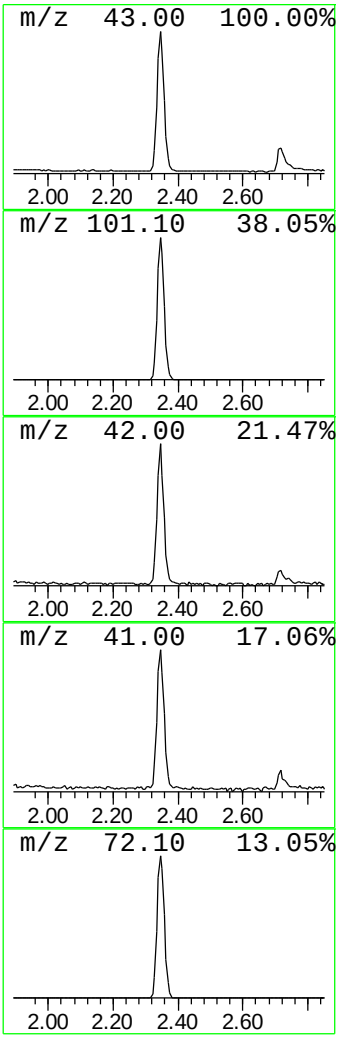
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.35	9.42 ng	408336	1,4-Dichlorobenzene-d4	6.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	64
2	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	33
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
4	Furazan-3-ol, 4-amino-	101	C2H3N3O2	159013-90-8	9
5	Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072417\
Data File : BF097009.D
Acq On : 25 Jul 2017 2:22
Operator : SJ/JU
Sample : I4361-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RAMP-D-1-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

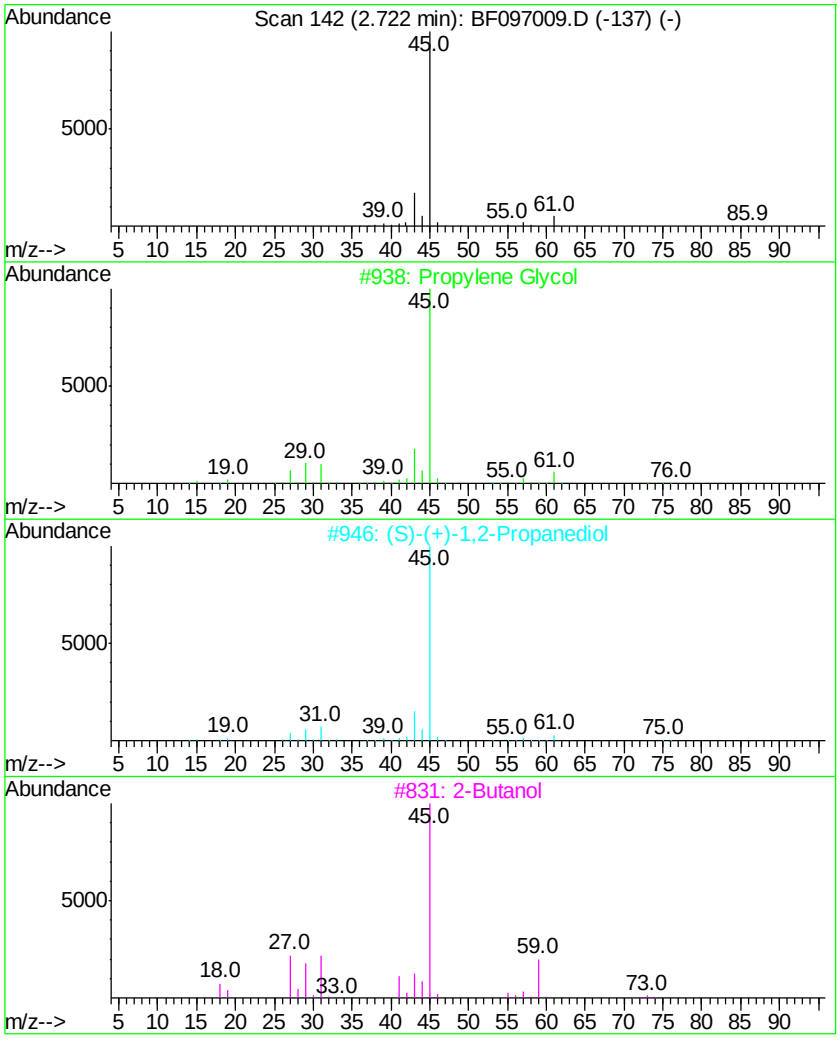
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

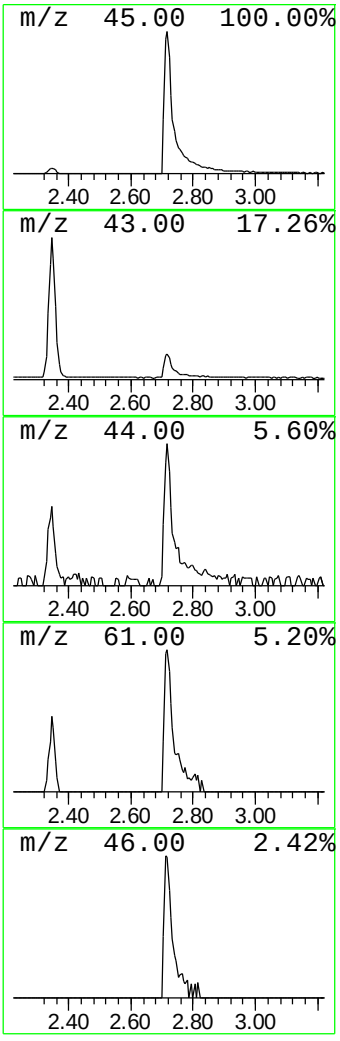
****

Peak Number 2 Propylene Glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.72	7.71 ng	334283	1,4-Dichlorobenzene-d4	6.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	74
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
3	2-Butanol	74	C4H10O	000078-92-2	9
4	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5	Formamide	45	CH3NO	000075-12-7	7





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072417\
Data File : BF097009.D
Acq On : 25 Jul 2017 2:22
Operator : SJ/JU
Sample : I4361-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RAMP-D-1-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

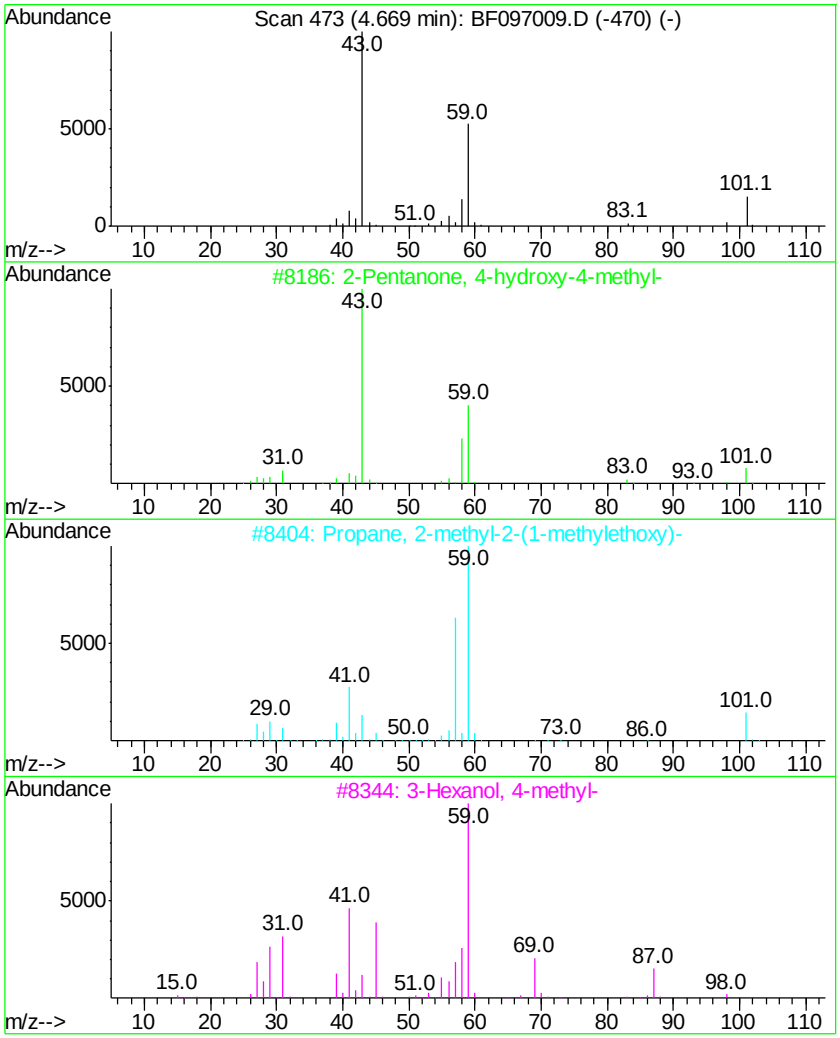
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

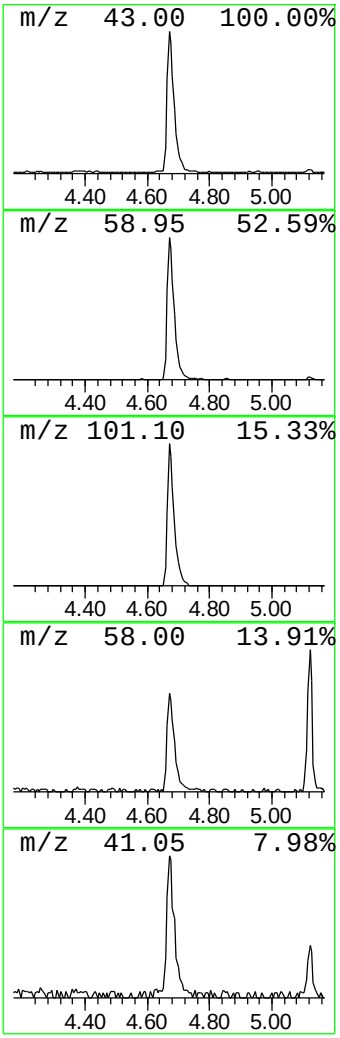
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.67	8.60 ng	372911	1,4-Dichlorobenzene-d4	6.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	3-Octanol	130	C8H18O	000589-98-0	33
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072417\
Data File : BF097009.D
Acq On : 25 Jul 2017 2:22
Operator : SJ/JU
Sample : I4361-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RAMP-D-1-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

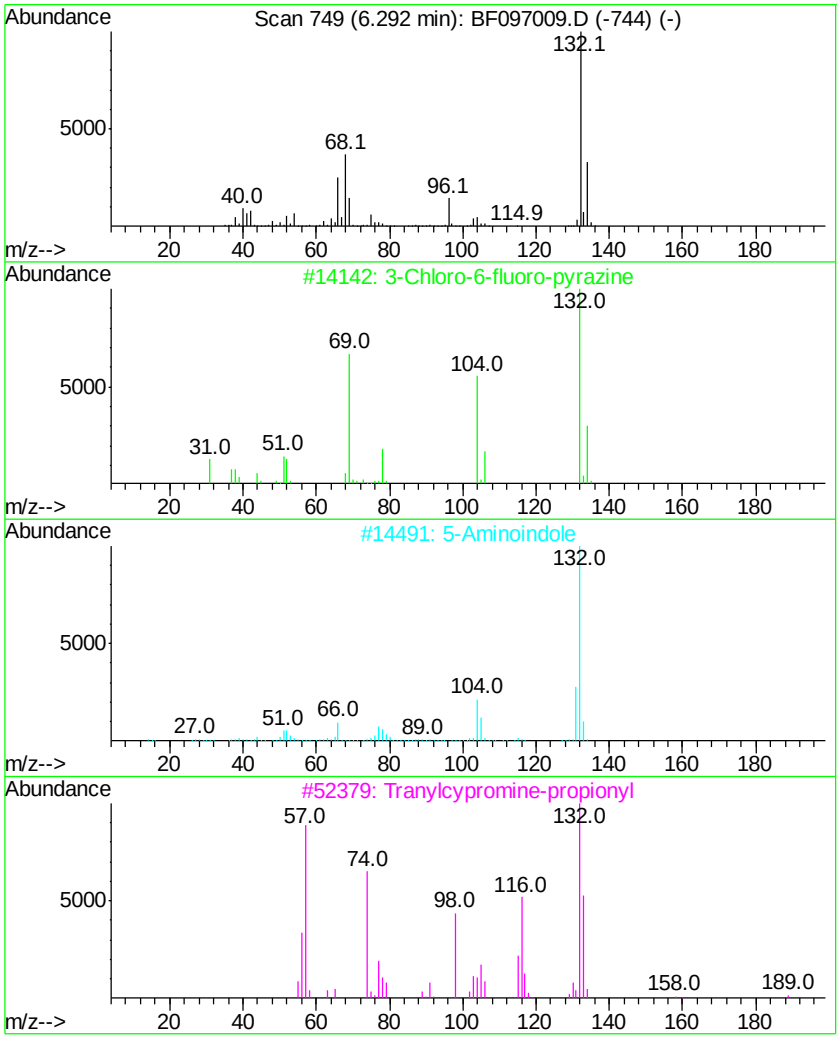
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

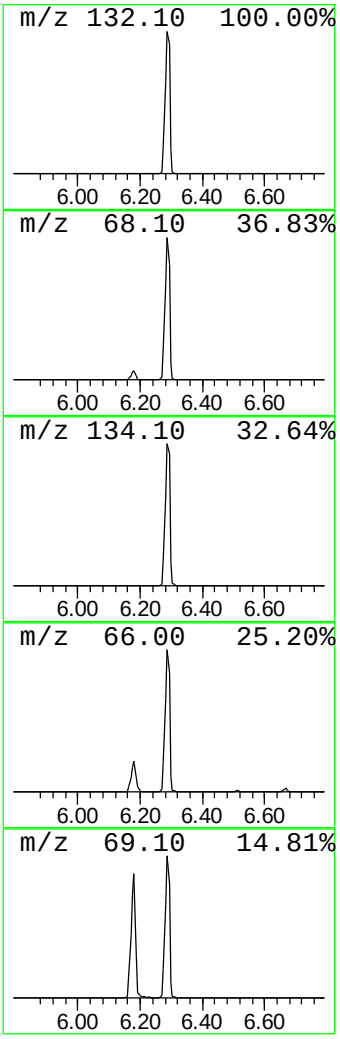
****

Peak Number 4 unknown6.29 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.29	72.20 ng	3131170	1,4-Dichlorobenzene-d4	6.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Sample : I4361-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RAMP-D-1-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

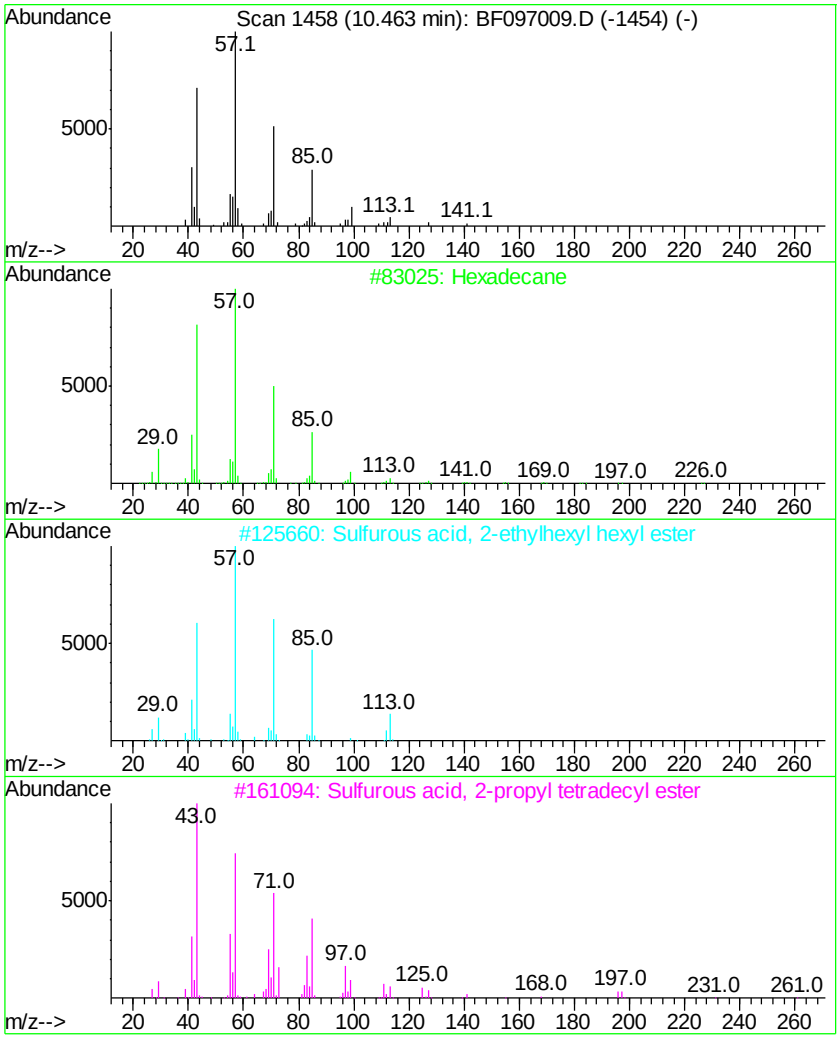
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

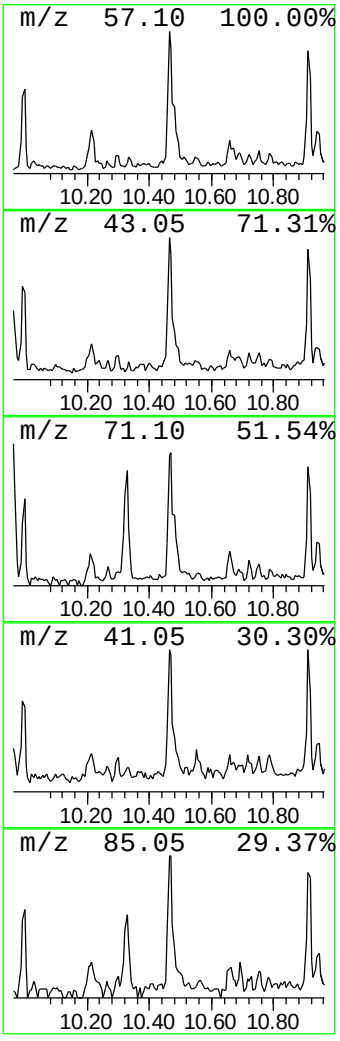
****

Peak Number 6 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.46	2.18 ng	114785	Phenanthrene-d10	11.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	80
3	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	80
4	Tetradecane	198	C14H30	000629-59-4	80
5	Tridecane	184	C13H28	000629-50-5	72





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072417\
Data File : BF097009.D
Acq On : 25 Jul 2017 2:22
Operator : SJ/JU
Sample : I4361-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RAMP-D-1-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

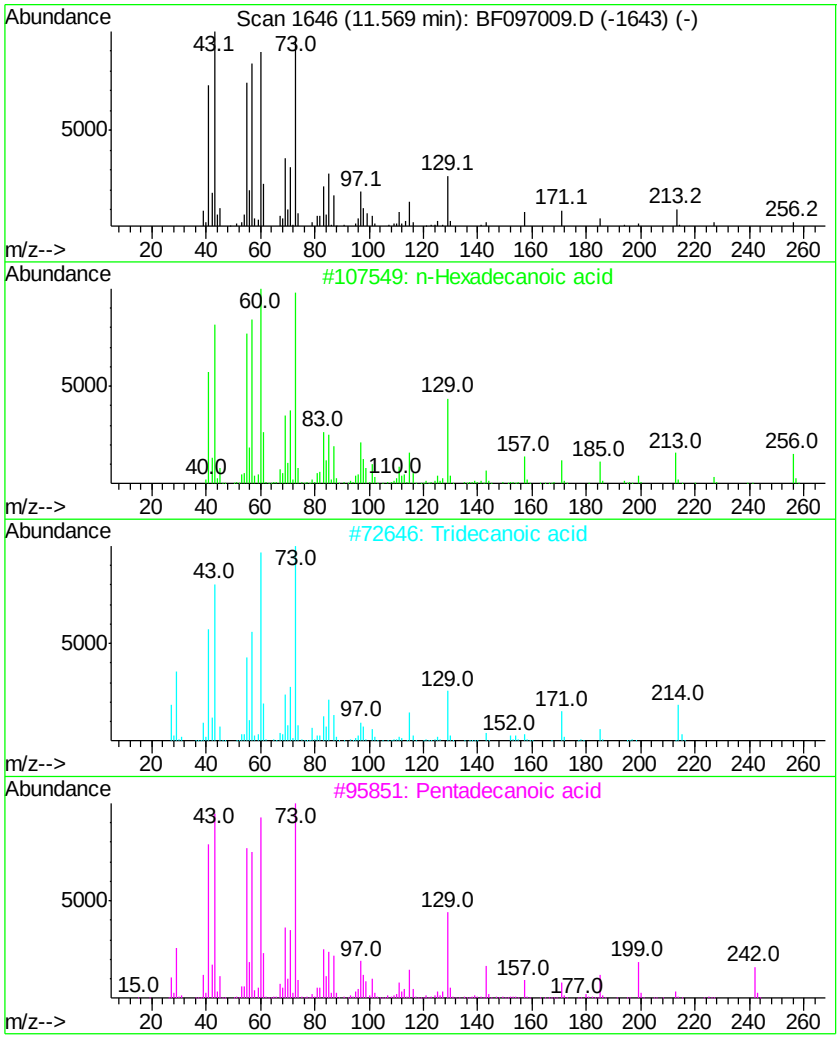
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

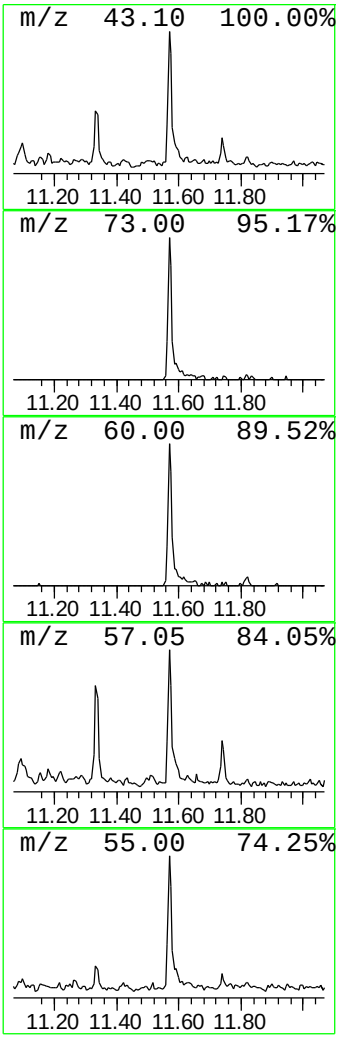
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.57	3.52 ng	185229	Phenanthrene-d10	11.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	97
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	59





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Sample : I4361-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RAMP-D-1-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

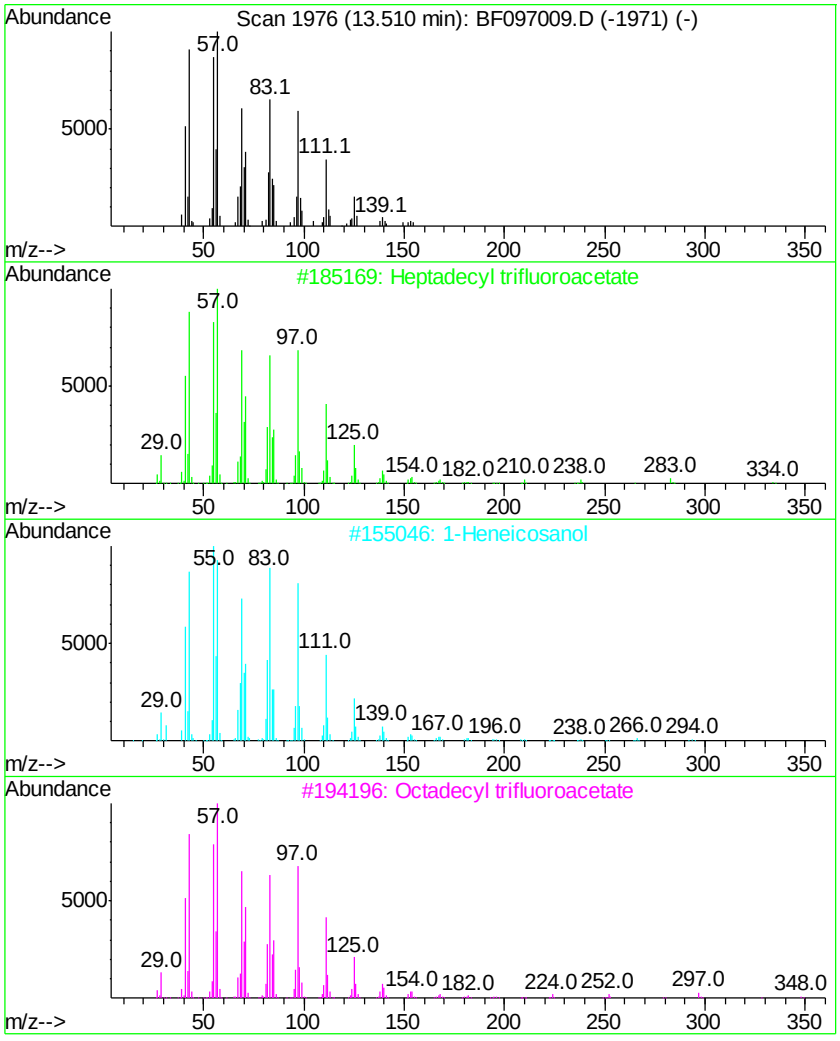
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

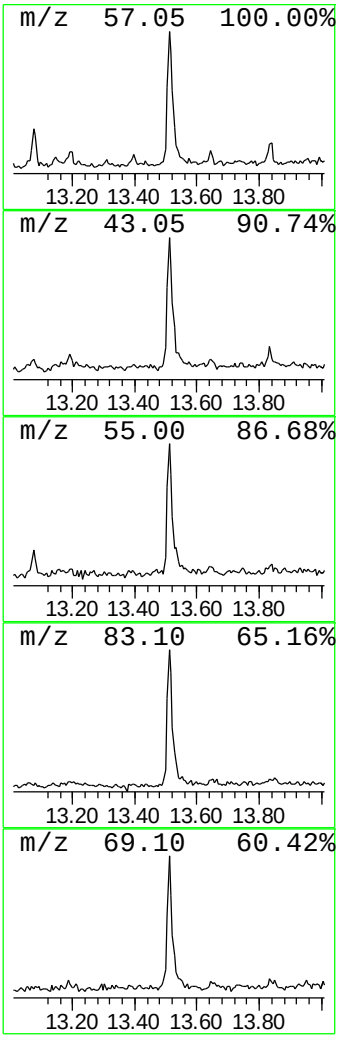
****

Peak Number 8 Heptadecyl trifluoroacetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.51	5.29 ng	207516	Chrysene-d12	13.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5	1-Docosene	308	C22H44	001599-67-3	91





Tentatively Identified Compound (LSC) summary

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Operator : SJ/JU
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
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
1,3-Dioxolane, 2,...	2.35	9.4	ng	408336	1	6.51	867301	20.0
Propylene Glycol	2.72	7.7	ng	334283	1	6.51	867301	20.0
2-Pentanone, 4-hy...	4.67	8.6	ng	372911	1	6.51	867301	20.0
unknown6.29	6.29	72.2	ng	3131170	1	6.51	867301	20.0
Hexadecane	10.46	2.2	ng	114785	4	11.02	1052190	20.0
n-Hexadecanoic acid	11.57	3.5	ng	185229	4	11.02	1052190	20.0
Heptadecyl triflu...	13.51	5.3	ng	207516	5	13.64	785282	20.0