LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022718\
Data File : BF103271.D
Acq On : 27 Feb 2018 18:55
Operator : SJ/JU
Sample : J1397-17
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-022318-E

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-BF022218.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	2.163	6	13	19	rBV	336924	449042	10.89%	1.333%
2	5.122	513	516	525	rBV	95934	142062	3.45%	0.422%
3	5.504	576	581	599	rBV	3644020	4123110	100.00%	12.243%
4	6.516	747	753	771	rBV	3388677	4057991	98.42%	12.049%
5	6.651	771	776	779	rBV	3801945	3837890	93.08%	11.396%
6	6.875	810	814	821	rBV	1165798	958496	23.25%	2.846%
7	7.034	836	841	844	rBV	3217129	3051340	74.01%	9.060%
8	7.439	905	910	913	rBV	2436559	2575120	62.46%	7.646%
9	7.534	923	926	936	rVB2	29047	49862	1.21%	0.148%
10	8.157	1028	1032	1048	rBV	1394719	1265487	30.69%	3.758%
11	8.651	1112	1116	1119	rVB	137997	109281	2.65%	0.324%
12	9.233	1210	1215	1218	rBV	3857283	3684222	89.36%	10.939%
13	9.569	1266	1272	1276	rBV	266338	250048	6.06%	0.742%
14	9.622	1276	1281	1289	rBV	406536	392546	9.52%	1.166%
15	9.833	1313	1317	1320	rBV	104704	92314	2.24%	0.274%
16	9.916	1327	1331	1338	rVB	1232086	1132215	27.46%	3.362%
17	10.304	1394	1397	1399	rBV	113609	84126	2.04%	0.250%
18	10.328	1399	1401	1404	rVB	123547	105941	2.57%	0.315%
19	10.551	1432	1439	1441	rBV	44276	53333	1.29%	0.158%
20	10.710	1461	1466	1474	rBV	1674656	1657603	40.20%	4.922%
21	10.804	1479	1482	1491	rVB	159484	172240	4.18%	0.511%
22	11.251	1555	1558	1561	rBV	110311	94943	2.30%	0.282%
23	11.280	1561	1563	1570	rVB2	42625	44112	1.07%	0.131%
24	11.404	1580	1584	1593	rBV	890119	928703	22.52%	2.758%
25	11.680	1628	1631	1634	rBV	97360	75648	1.83%	0.225%
26	12.086	1697	1700	1704	rBV	68864	57121	1.39%	0.170%
27	12.621	1788	1791	1797	rVB	51349	50820	1.23%	0.151%
28	12.851	1825	1830	1832	rBV	51562	61488	1.49%	0.183%
29	12.992	1849	1854	1857	rBV	2571193	2465601	59.80%	7.321%
30	13.868	2000	2003	2015	rBV	147112	224245	5.44%	0.666%
31	14.057	2030	2035	2046	rBV	790459	890163	21.59%	2.643%
32	15.557	2286	2290	2299	rVB	389059	541209	13.13%	1.607%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022718\
Data File : BF103271.D
Acq On : 27 Feb 2018 18:55
Operator : SJ/JU
Sample : J1397-17
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-022318-E

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-BF022218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 33678322

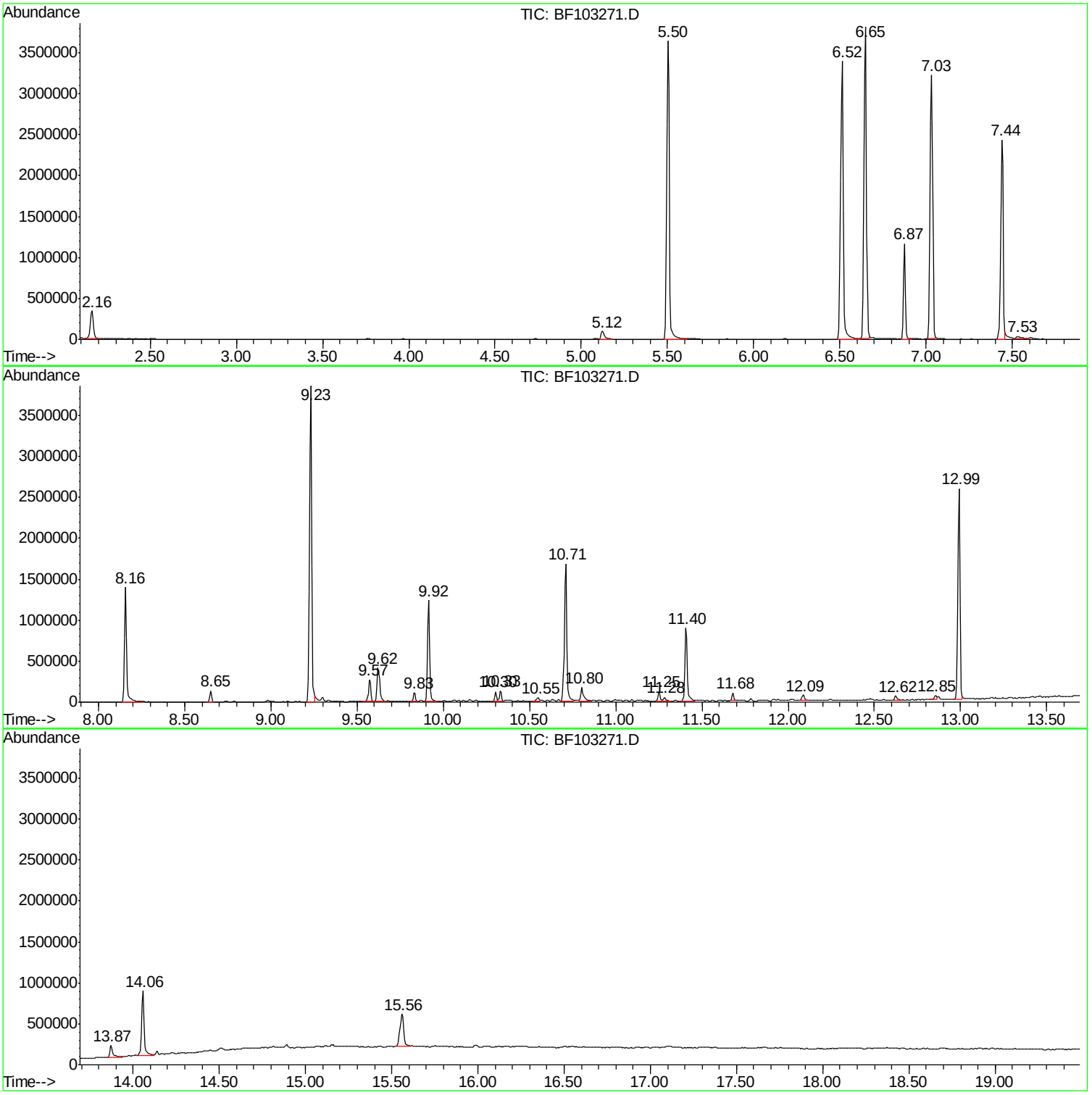
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022718\
Data File : BF103271.D
Acq On : 27 Feb 2018 18:55
Operator : SJ/JU
Sample : J1397-17
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-022318-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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\BF022718\
Data File : BF103271.D
Acq On : 27 Feb 2018 18:55
Operator : SJ/JU
Sample : J1397-17
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-022318-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

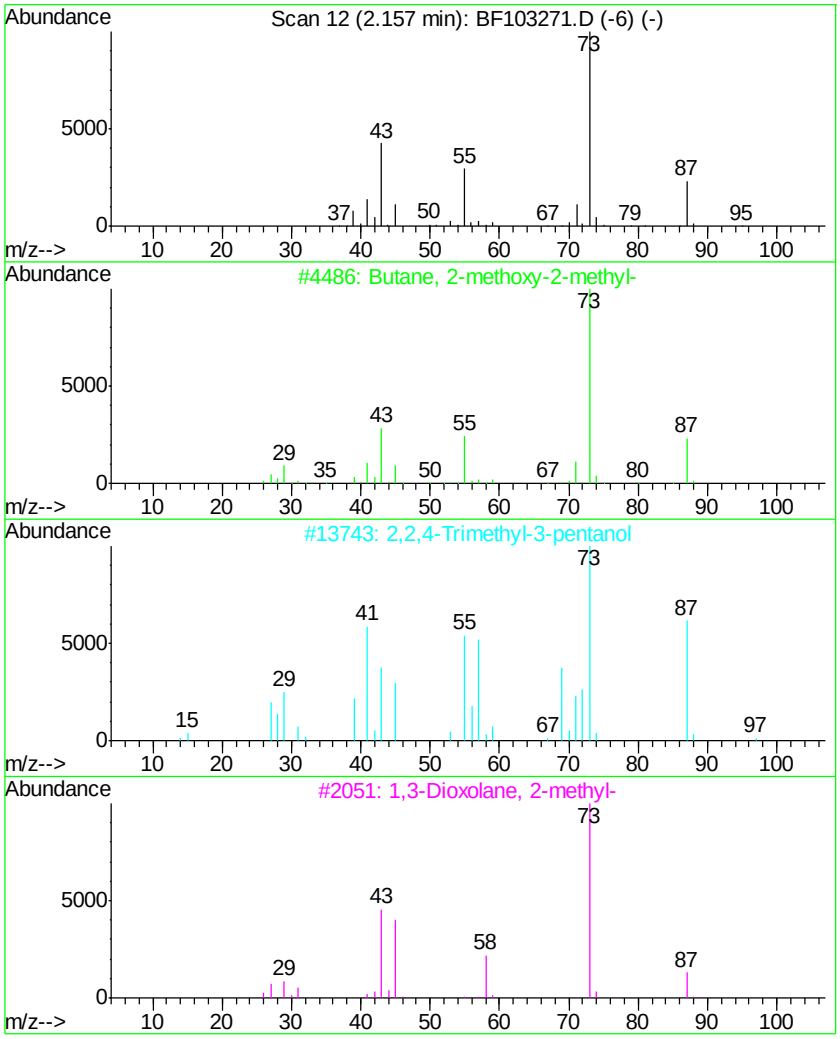
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

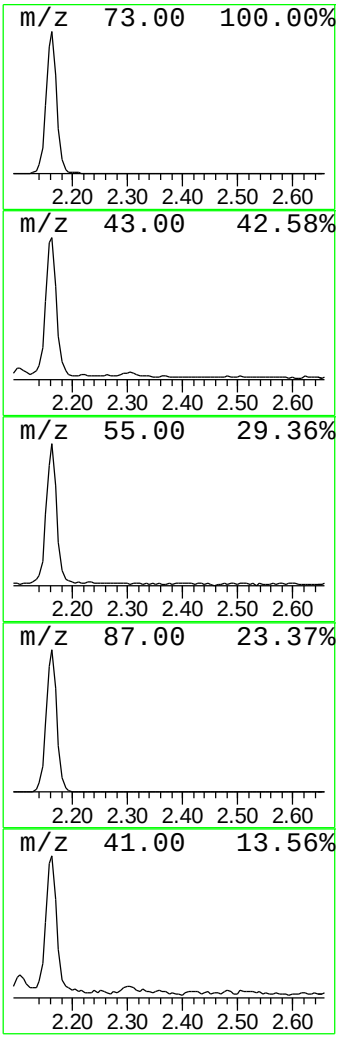
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	9.37 ng	449042	1,4-Dichlorobenzene-d4	6.87

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\HPCHEM1\BNA F\DATA\BF022718\
Data File : BF103271.D
Acq On : 27 Feb 2018 18:55
Operator : SJ/JU
Sample : J1397-17
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-022318-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

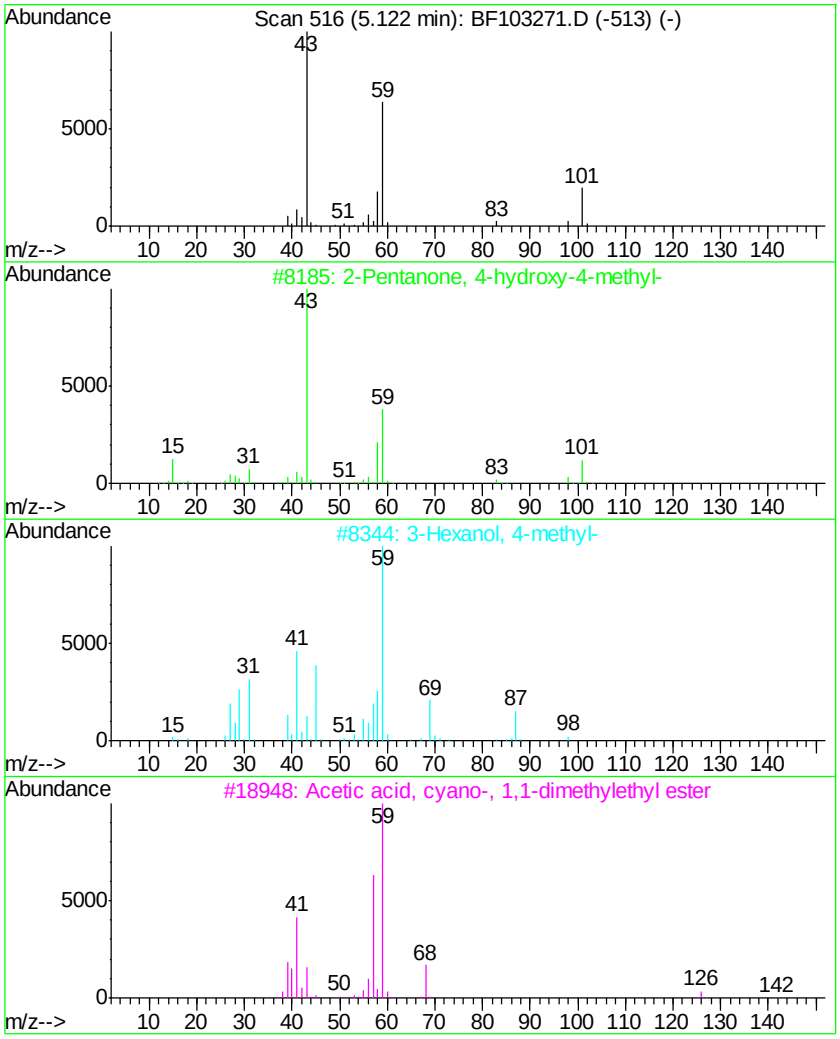
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

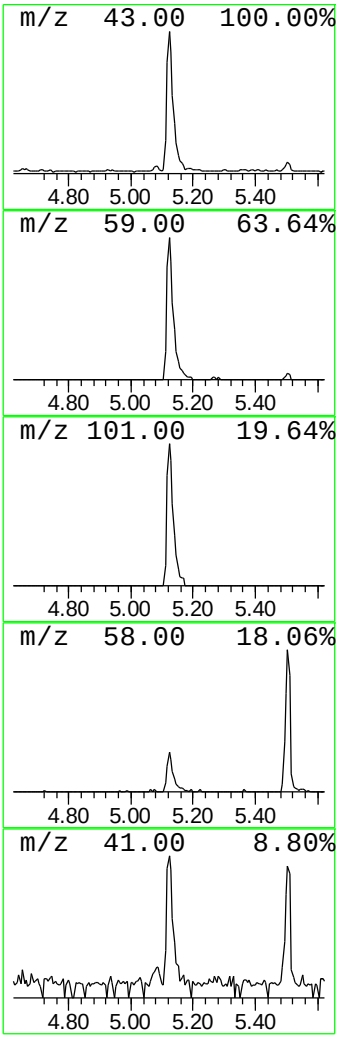
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	2.96 ng	142062	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Acetone	58	C3H6O	000067-64-1	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF022718\
Data File : BF103271.D
Acq On : 27 Feb 2018 18:55
Operator : SJ/JU
Sample : J1397-17
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-022318-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

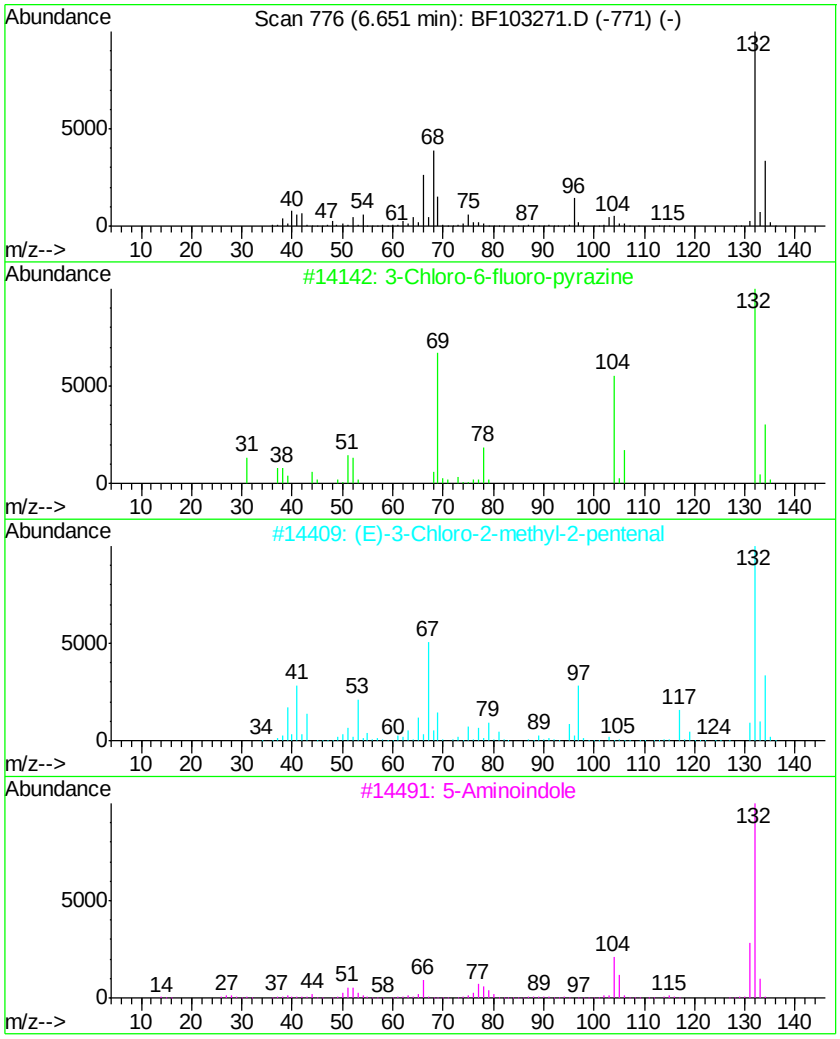
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

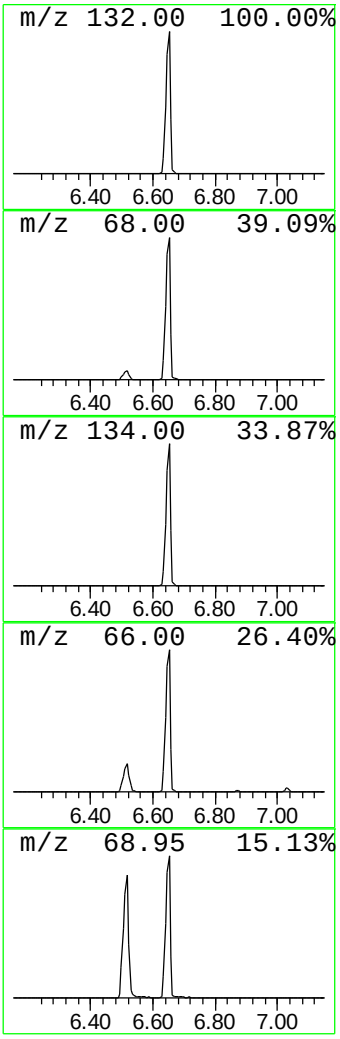
****

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	80.08 ng	3837890	1,4-Dichlorobenzene-d4	6.87

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





Data Path : Z:\HPCHEM1\BNA F\DATA\BF022718\
Data File : BF103271.D
Acq On : 27 Feb 2018 18:55
Operator : SJ/JU
Sample : J1397-17
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-022318-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

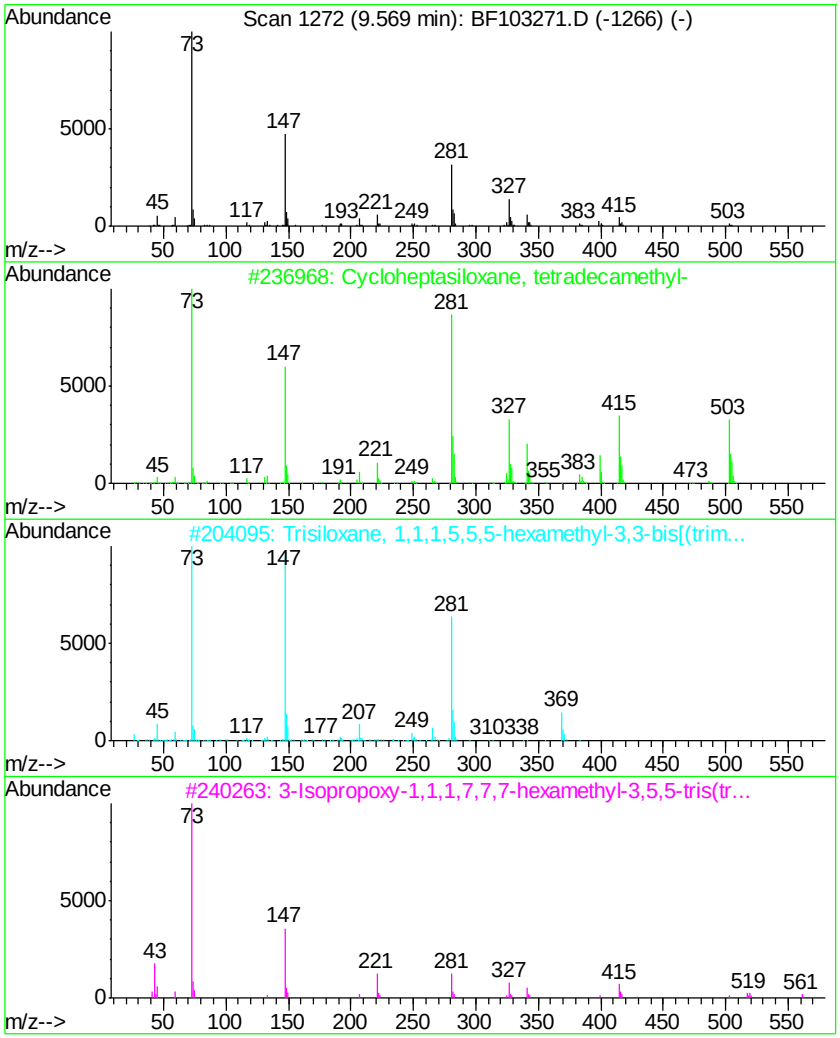
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

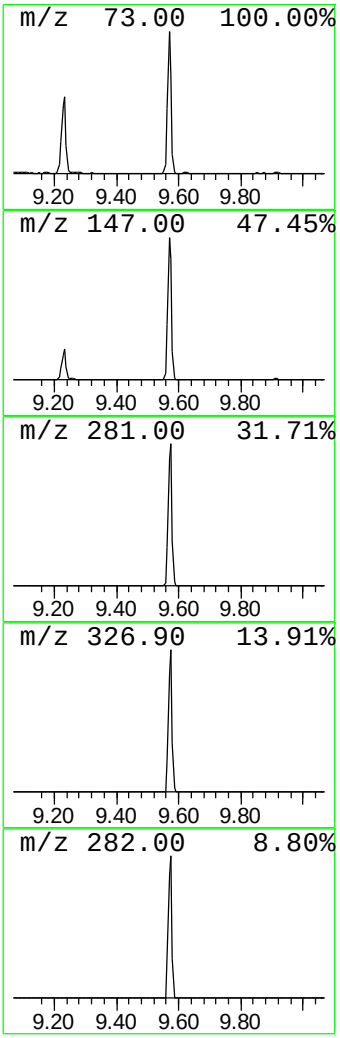
****

Peak Number 5 Cycloheptasiloxane, tetrade... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.57	4.42 ng	250048	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloheptasiloxane, tetradecamet...	518	C14H42O7Si7	000107-50-6	91
2	Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	59
3	3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	50
4	Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	43
5	Propanedioic acid, [(trimethylsi...	336	C12H28O5Si3	038165-93-4	37





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Acq On : 27 Feb 2018 18:55
Operator : SJ/JU
Sample : J1397-17
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-022318-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

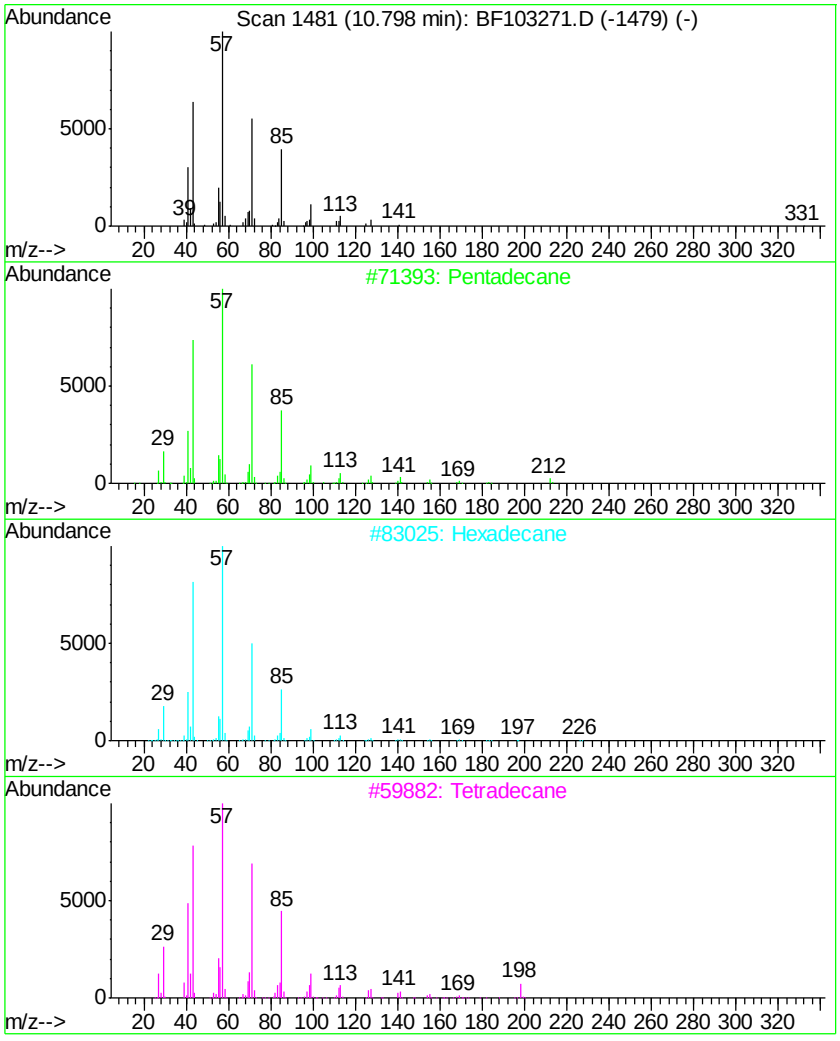
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

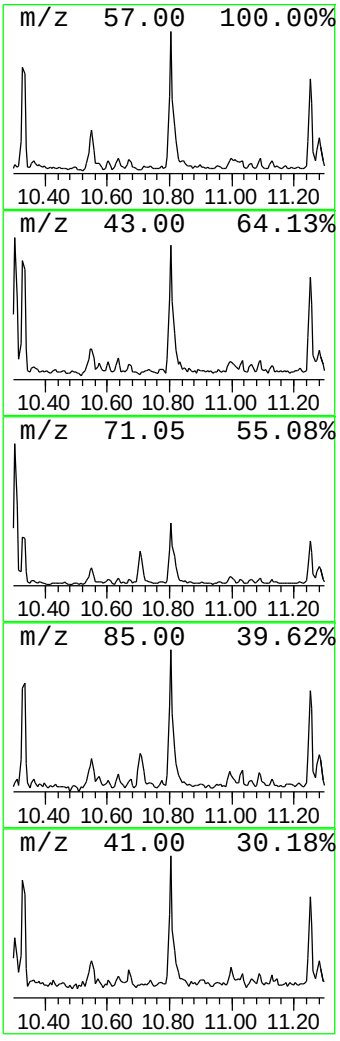
****

Peak Number 6 Pentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	3.71 ng	172240	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Tetradecane	198	C14H30	000629-59-4	86
4	Tridecane	184	C13H28	000629-50-5	83
5	Bacchotricuneatin c	342	C20H22O5	066563-30-2	76





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Operator : SJ/JU
Sample : J1397-17
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-022318-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

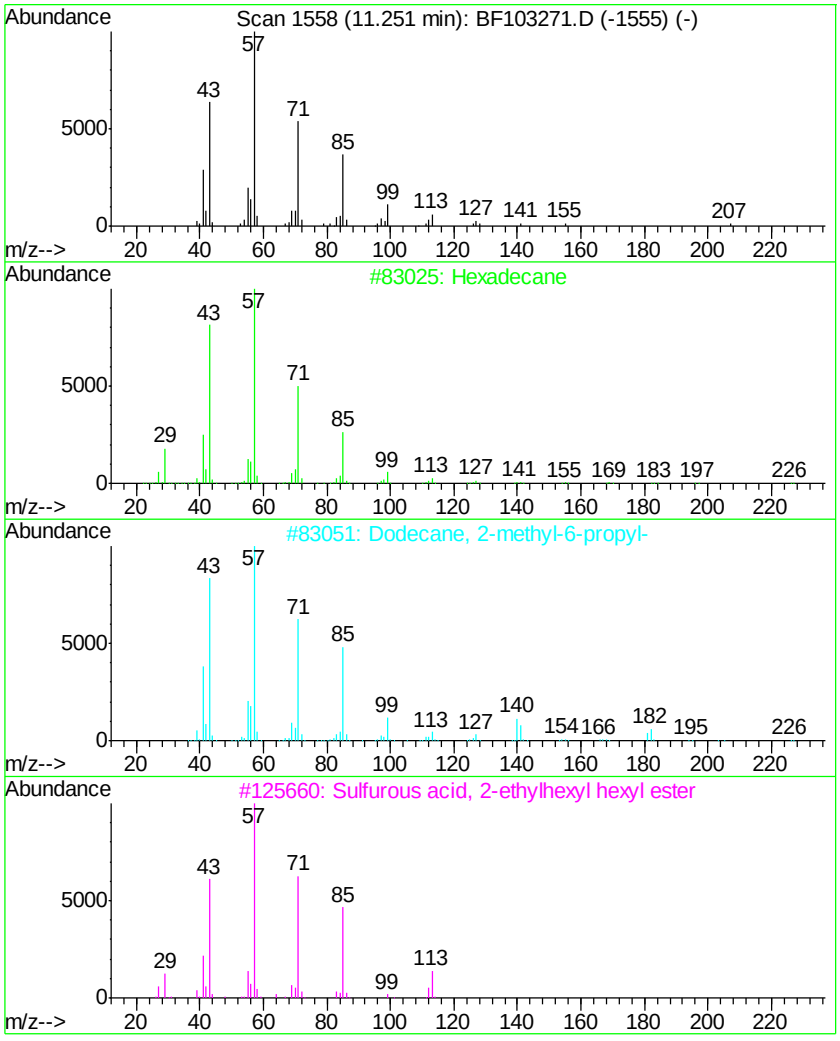
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

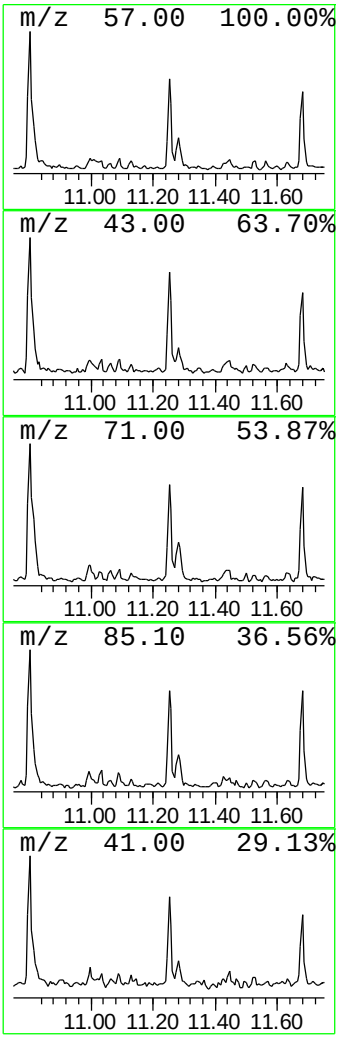
****

Peak Number 7 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.25	2.04 ng	94943	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86
3	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	72
4	Tridecane, 7-propyl-	226	C16H34	055045-09-5	72
5	Bacchotricuneatin c	342	C20H22O5	066563-30-2	68





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Acq On : 27 Feb 2018 18:55
Operator : SJ/JU
Sample : J1397-17
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-022318-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

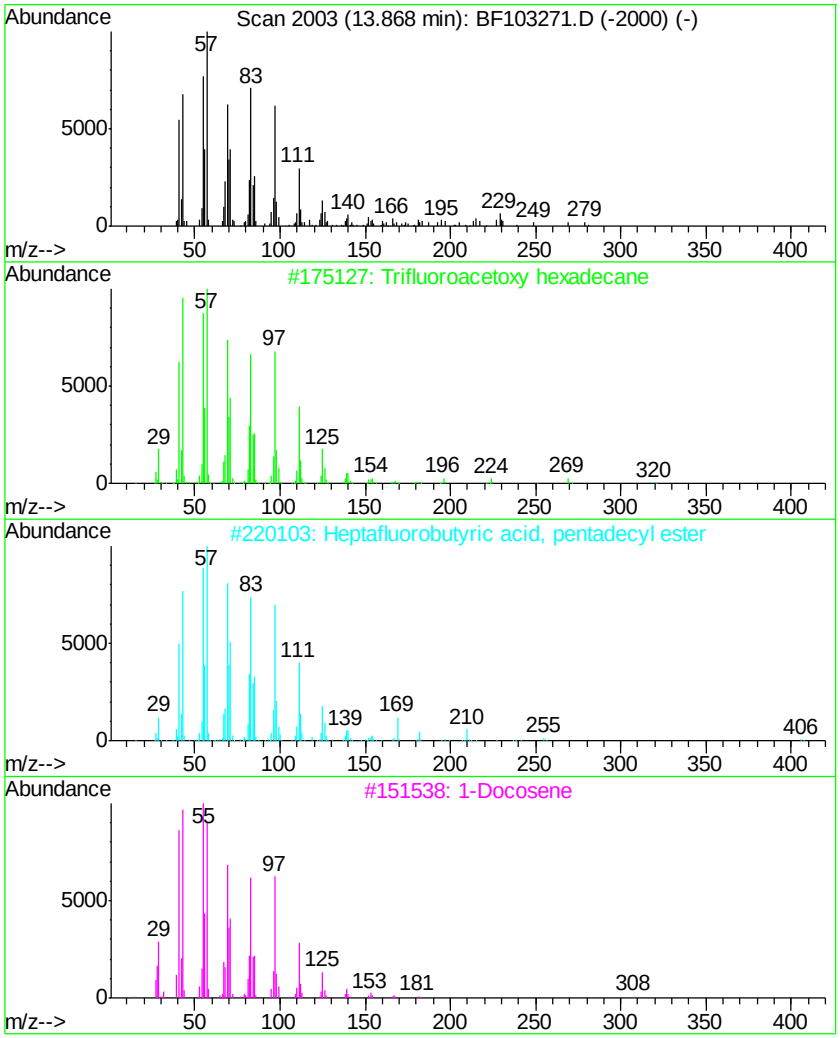
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

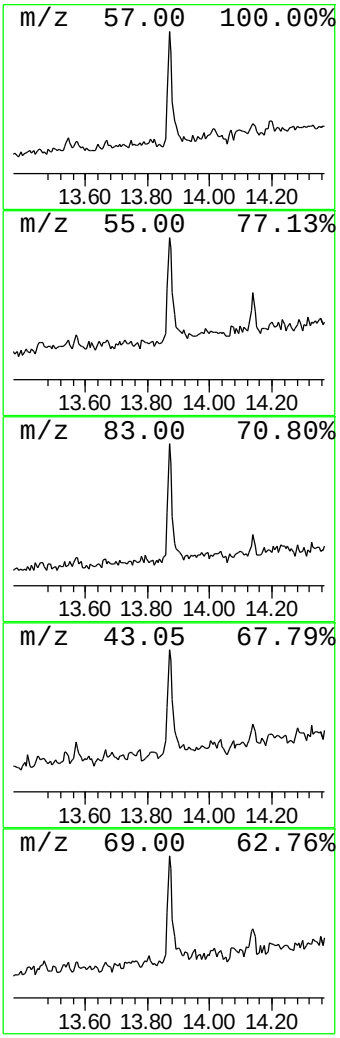
****

Peak Number 8 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	5.04 ng	224245	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	1-Docosene	308	C22H44	001599-67-3	94
4	Cyclotridecane	182	C13H26	000295-02-3	93
5	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022718\
Data File : BF103271.D
Acq On : 27 Feb 2018 18:55
Operator : SJ/JU
Sample : J1397-17
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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
Butane, 2-methoxy...	2.16	9.4	ng	449042	1	6.87	958496	20.0
2-Pentanone, 4-hy...	5.12	3.0	ng	142062	1	6.87	958496	20.0
unknown6.65	6.65	80.1	ng	3837890	1	6.87	958496	20.0
Cycloheptasiloxan...	9.57	4.4	ng	250048	3	9.92	1132220	20.0
Pentadecane	10.80	3.7	ng	172240	4	11.40	928703	20.0
Hexadecane	11.25	2.0	ng	94943	4	11.40	928703	20.0
Trifluoroacetoxy ...	13.87	5.0	ng	224245	5	14.06	890163	20.0