LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA F\Data\BF122819\
Data File : BF118376.D
Acq On : 28 Dec 2019 20:21
Operator : JU
Sample : K6439-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIED-BF003-01

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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	5.063	502	506	522	rVB	451345	614688	10.93%	1.636%
2	5.475	571	576	586	rBV	3427460	3250304	57.77%	8.652%
3	6.492	744	749	767	rBV	3389965	3520721	62.58%	9.372%
4	6.628	767	772	775	rBV	3875454	3746565	66.59%	9.973%
5	6.851	806	810	819	rVB	788642	647637	11.51%	1.724%
6	7.010	833	837	840	rBV	3360911	2866078	50.94%	7.629%
7	7.416	902	906	931	rBV	2055413	2216634	39.40%	5.900%
8	8.139	1025	1029	1048	rBV	848796	841164	14.95%	2.239%
9	9.216	1208	1212	1215	rBV	5204722	4434520	78.82%	11.804%
10	9.610	1276	1279	1290	rBV	253904	275448	4.90%	0.733%
11	9.898	1324	1328	1341	rBV	1156133	1026480	18.24%	2.732%
12	10.692	1459	1463	1476	rBV	3243518	3294008	58.55%	8.768%
13	11.392	1578	1582	1590	rBV	1220366	1113560	19.79%	2.964%
14	11.916	1667	1671	1693	rBV	343352	395209	7.02%	1.052%
15	12.704	1802	1805	1811	rBV2	58571	74762	1.33%	0.199%
16	12.986	1848	1853	1856	rBV	6012599	5626260	100.00%	14.976%
17	13.874	2000	2004	2017	rBV	408593	661879	11.76%	1.762%
18	14.045	2029	2033	2041	rBV	1131182	1106204	19.66%	2.945%
19	14.498	2107	2110	2113	rBV	82793	89155	1.58%	0.237%
20	14.810	2157	2163	2168	rBV2	110554	150380	2.67%	0.400%
21	15.151	2217	2221	2226	rBV	120818	138481	2.46%	0.369%
22	15.539	2282	2287	2294	rBV	858252	1111346	19.75%	2.958%
23	15.980	2357	2362	2368	rBV2	85530	125235	2.23%	0.333%
24	16.056	2369	2375	2389	rVV9	48769	148792	2.64%	0.396%
25	16.492	2443	2449	2454	rBV2	53910	92787	1.65%	0.247%

Sum of corrected areas: 37568297

LSC Report - Integrated Chromatogram

Data Path : Z:\svoasrv\HPCHEM1\BNA F\Data\BF122819\
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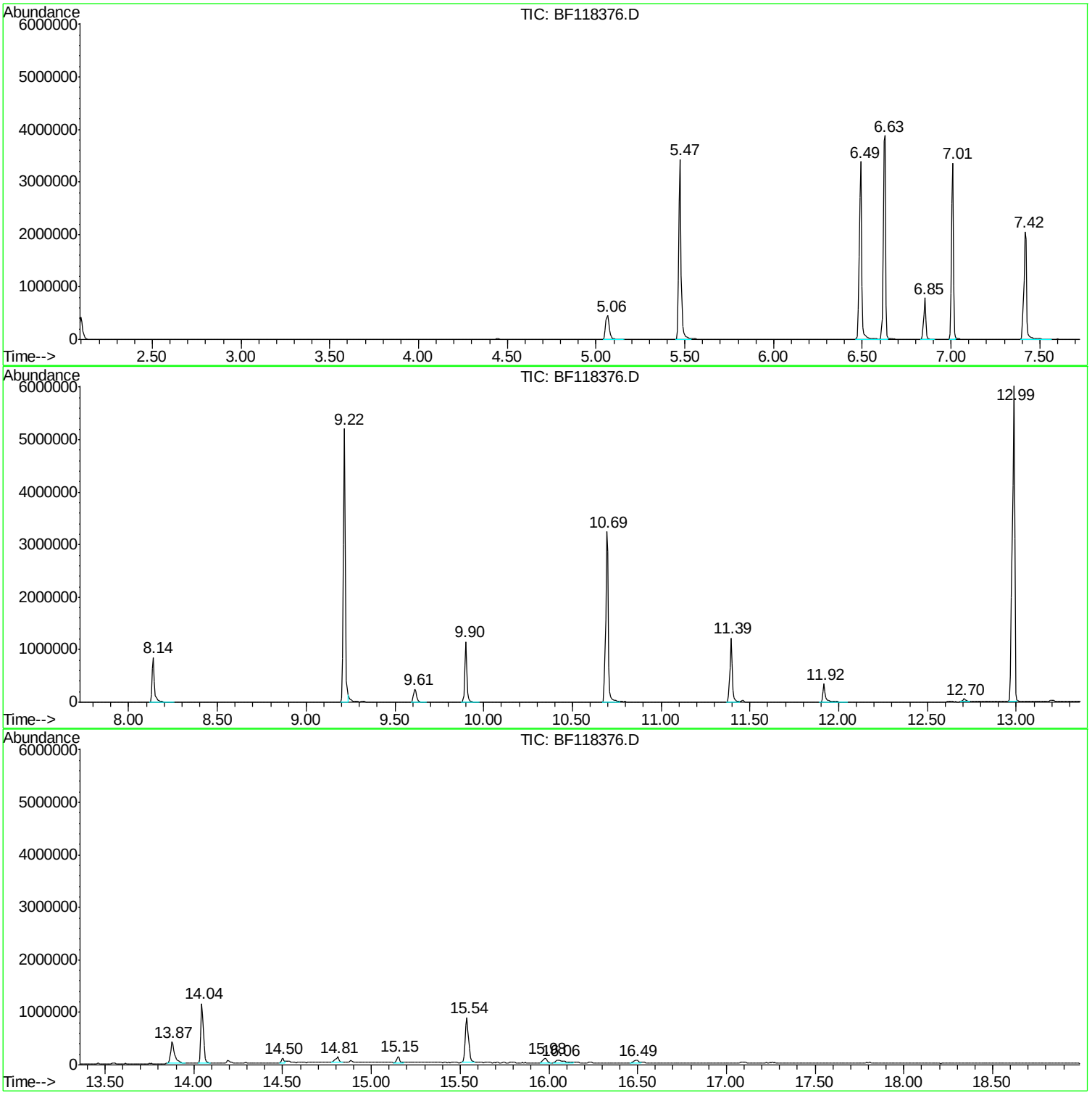
Acq On : 28 Dec 2019 20:21
Operator : JU
Sample : K6439-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LIED-BF003-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\svoasrv\HPCHEM1\BNA F\Data\BF122819\
Data File : BF118376.D
Acq On : 28 Dec 2019 20:21
Operator : JU
Sample : K6439-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIED-BF003-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

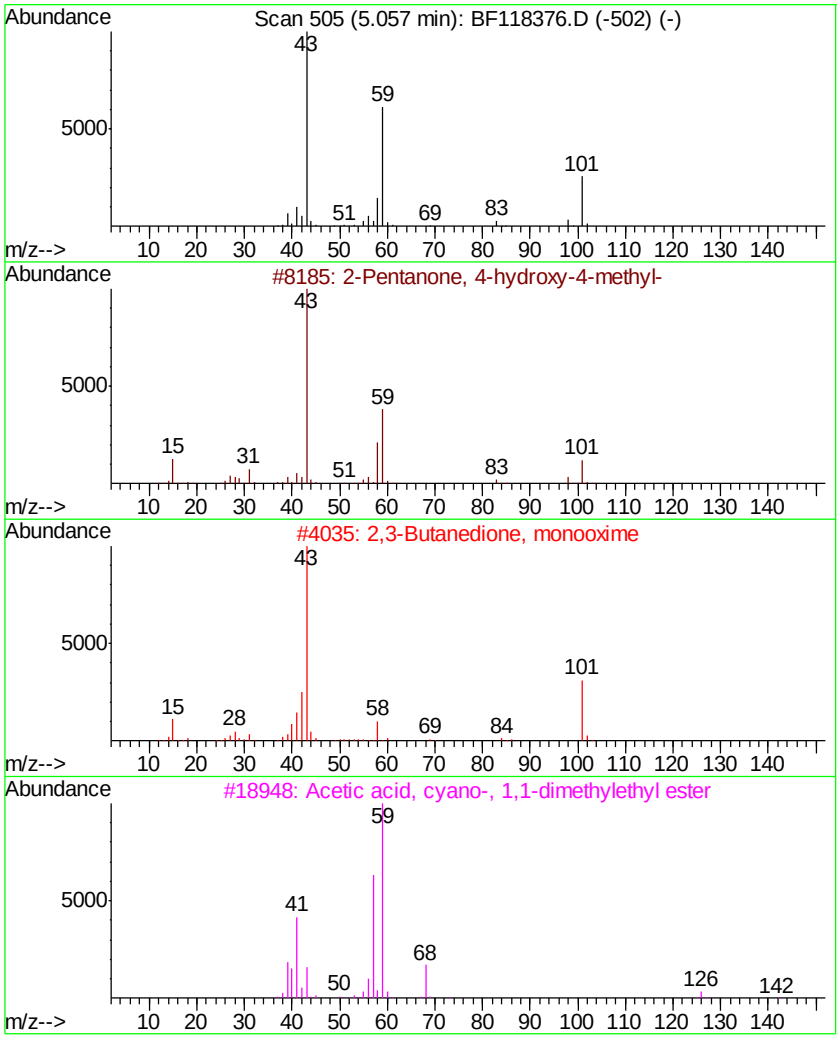
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

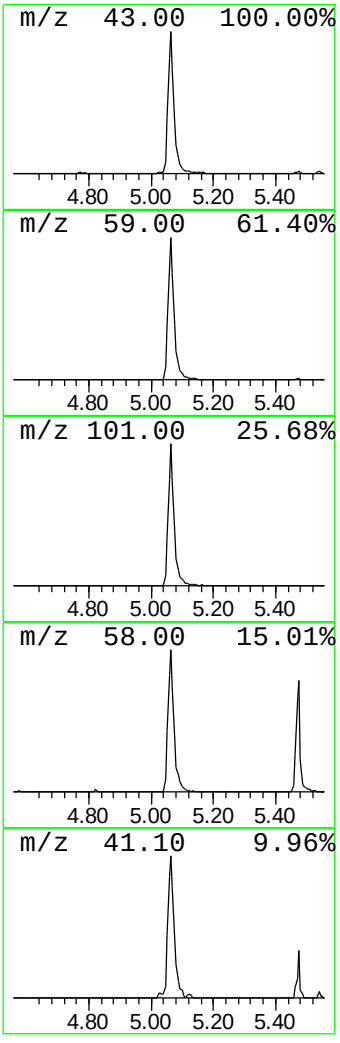
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	18.98 ng	614688	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

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Data File : BF118376.D
Acq On : 28 Dec 2019 20:21
Operator : JU
Sample : K6439-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIED-BF003-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

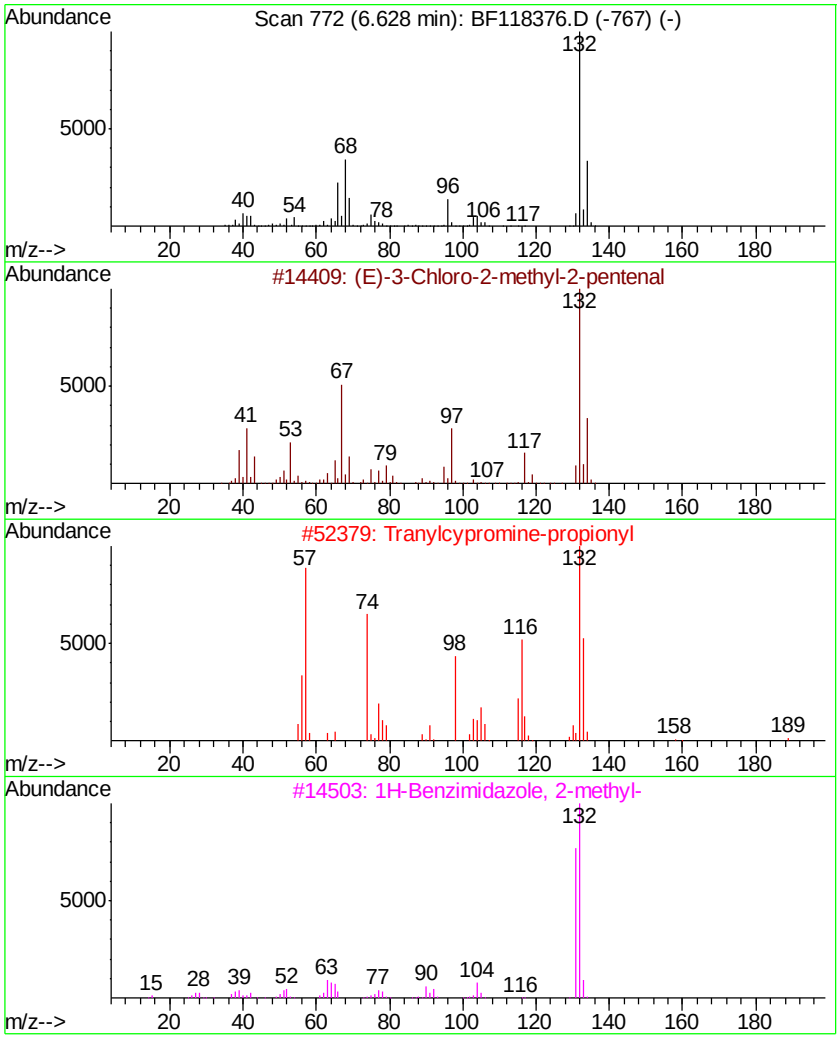
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

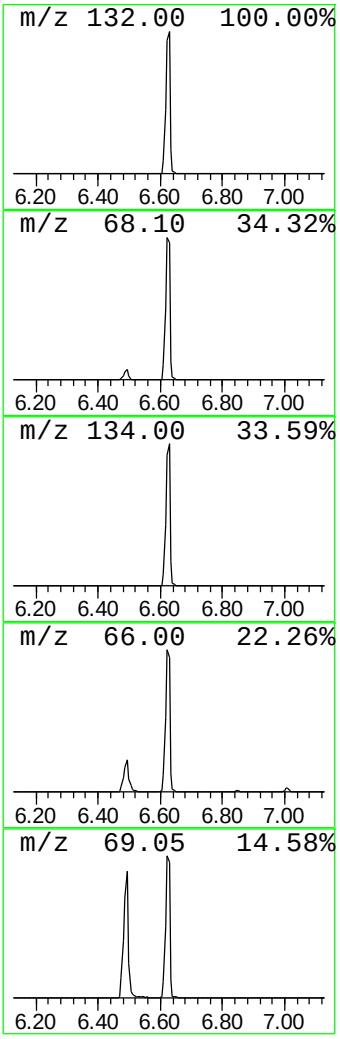
****

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	115.70 ng	3746570	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9





Library Search Compound Report

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Acq On : 28 Dec 2019 20:21
Operator : JU
Sample : K6439-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIED-BF003-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

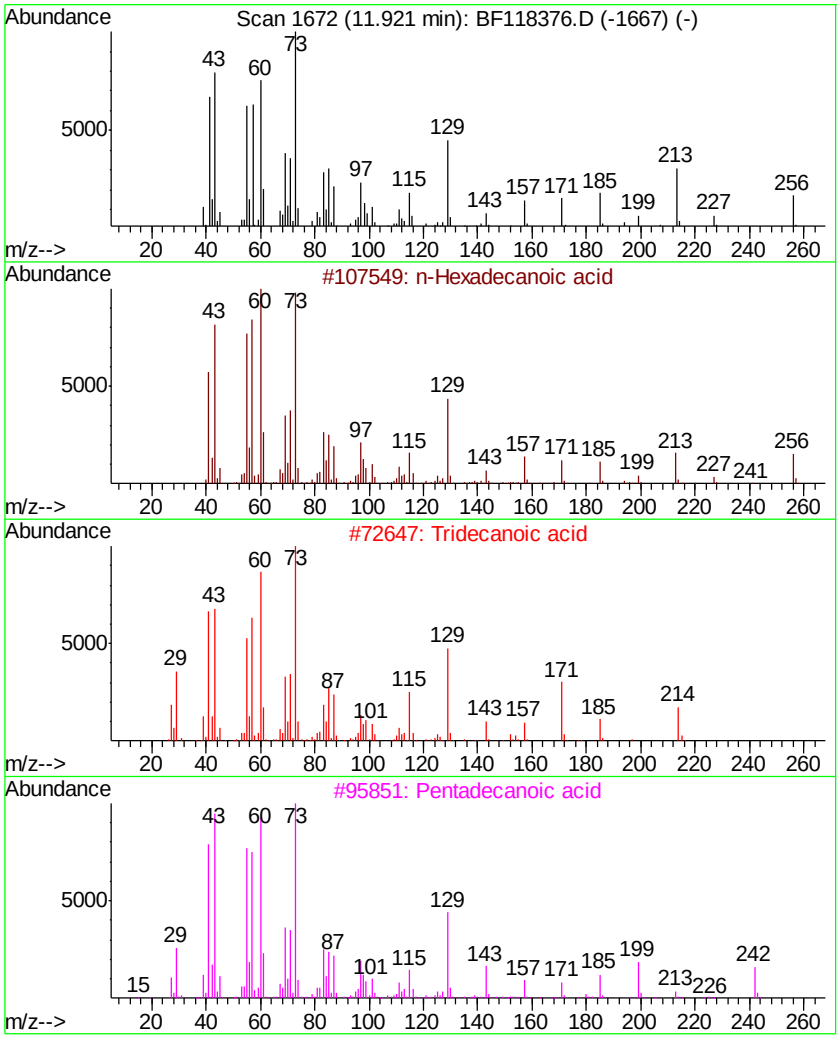
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

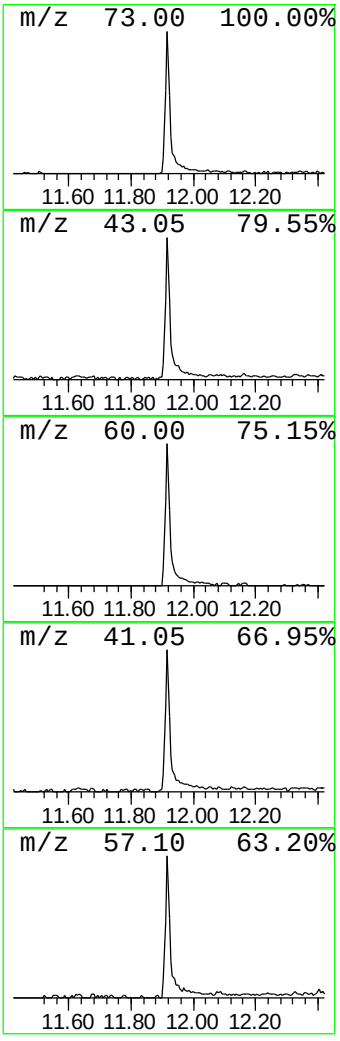
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	7.10 ng	395209	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





Data Path : Z:\svoasrv\HPCHEM1\BNA F\Data\BF122819\
Data File : BF118376.D
Acq On : 28 Dec 2019 20:21
Operator : JU
Sample : K6439-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIED-BF003-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

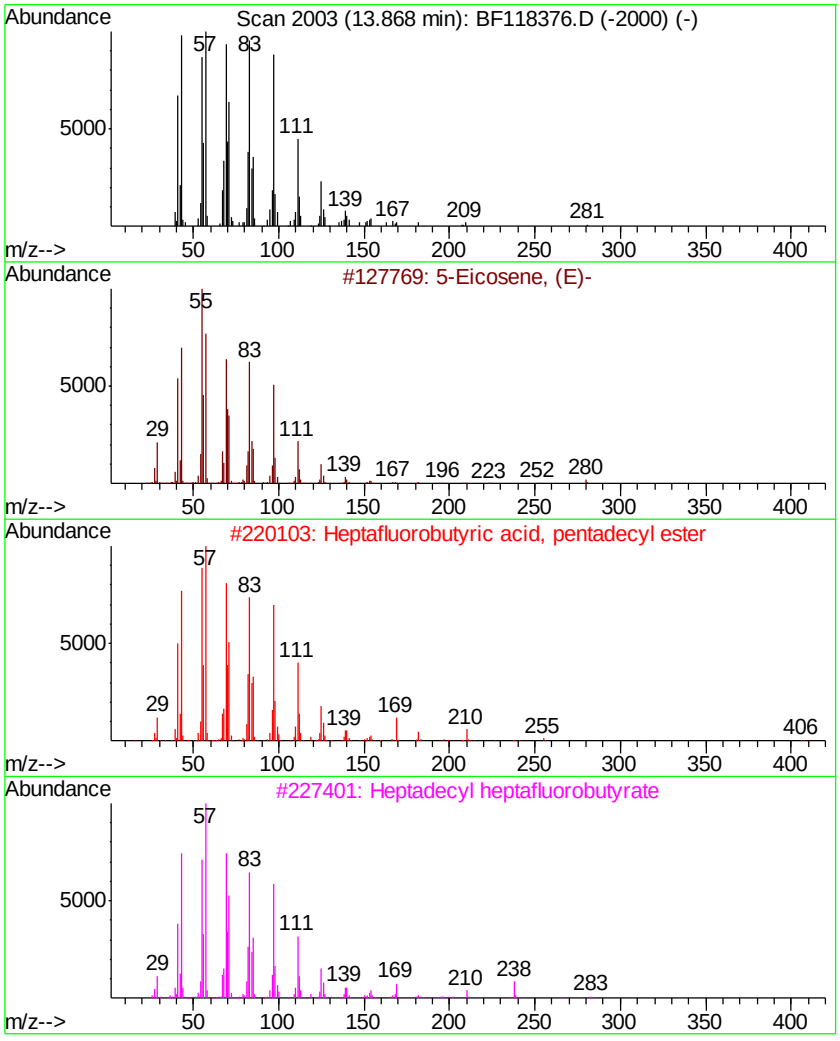
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

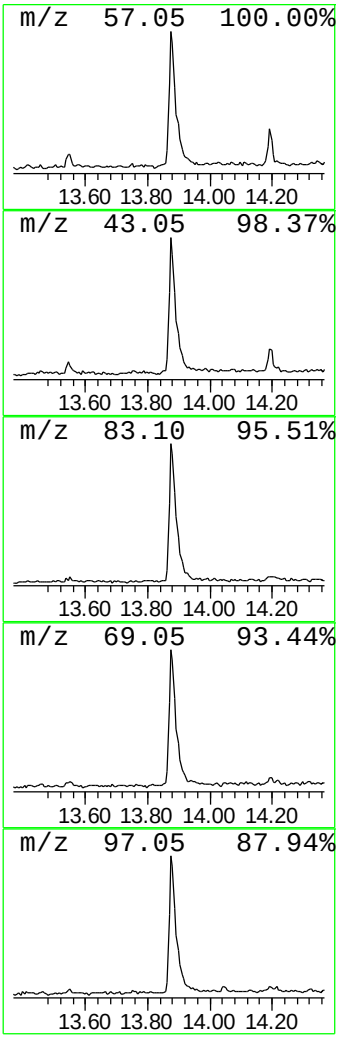
****

Peak Number 5 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	11.97 ng	661879	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94





Library Search Compound Report

Data Path : Z:\svoasrv\HPCHEM1\BNA F\Data\BF122819\
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Instrument : BNA_F
ClientSampleId : LIED-BF003-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

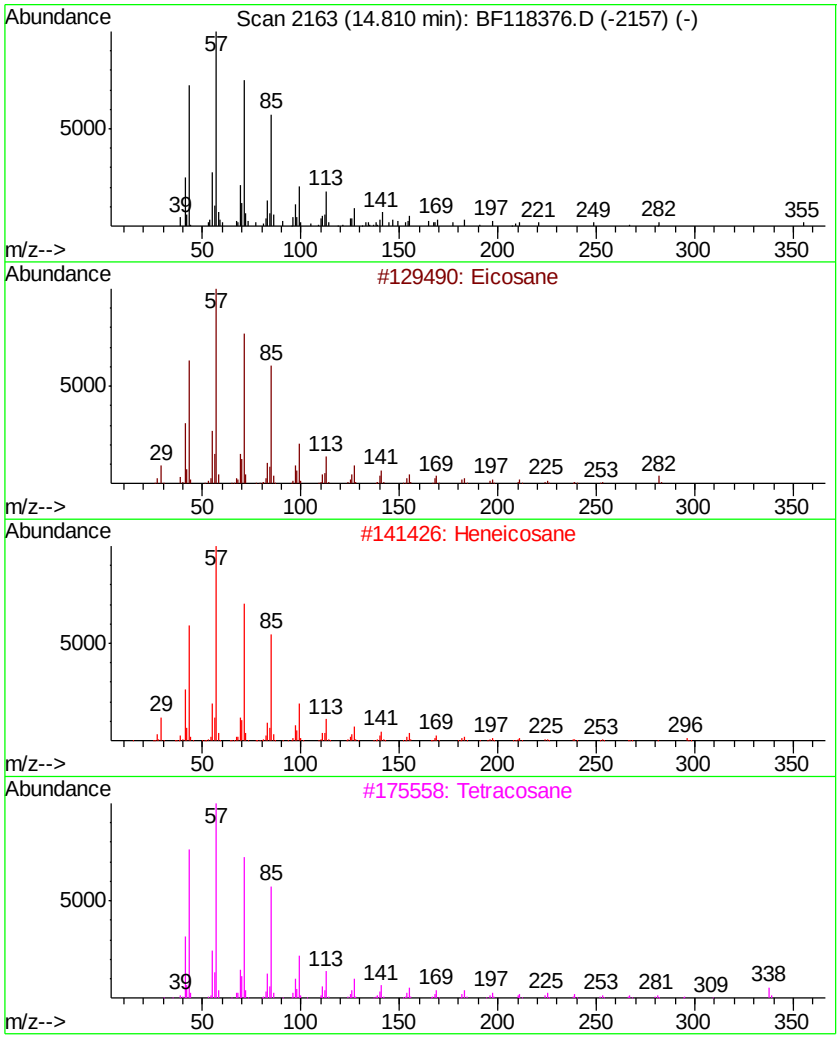
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

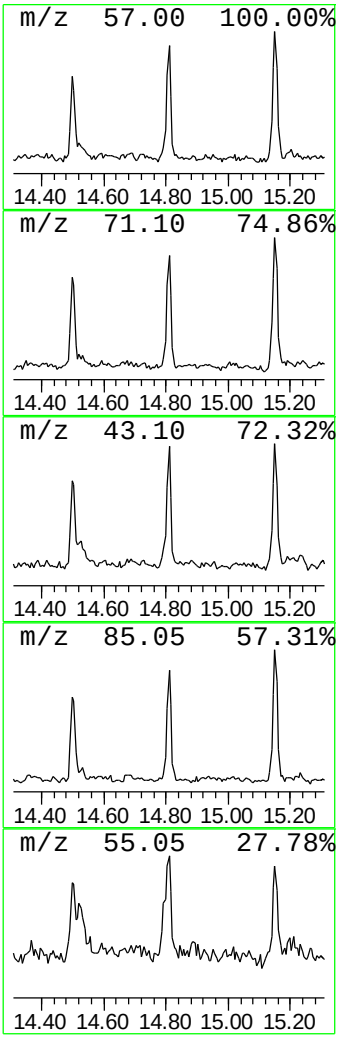
****

Peak Number 6 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	2.71 ng	150380	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Docosane	310	C22H46	000629-97-0	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Library Search Compound Report

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Operator : JU
Sample : K6439-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIED-BF003-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

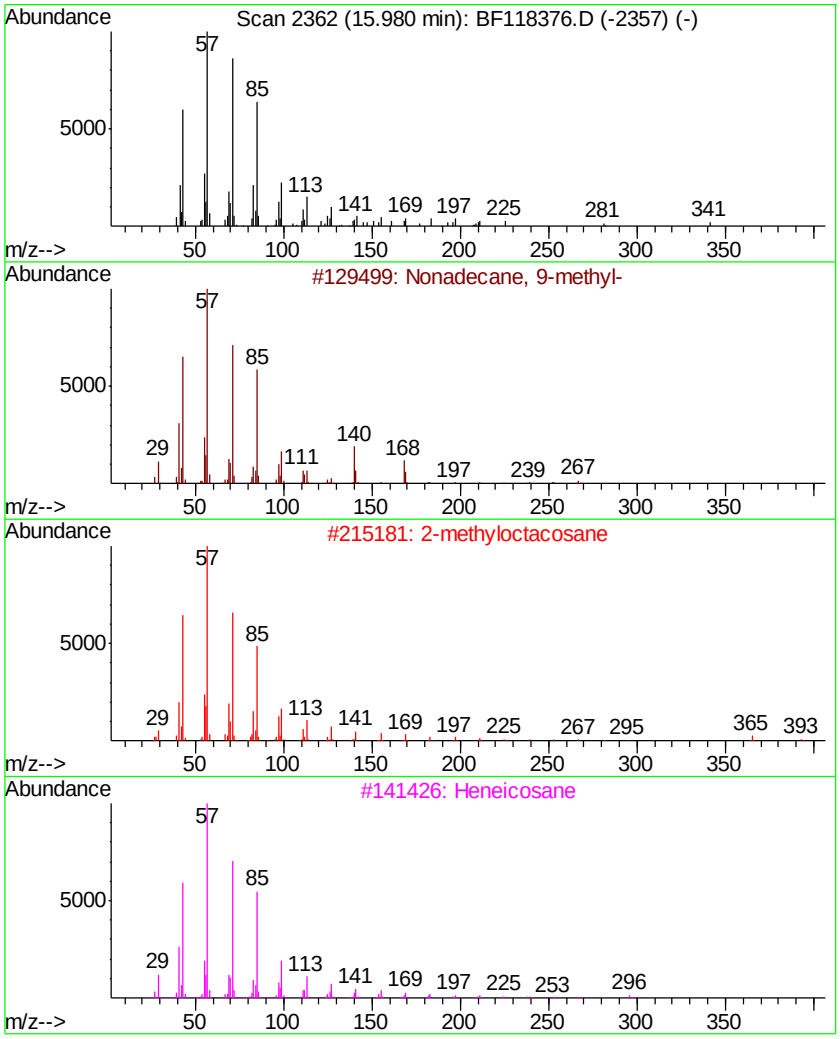
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

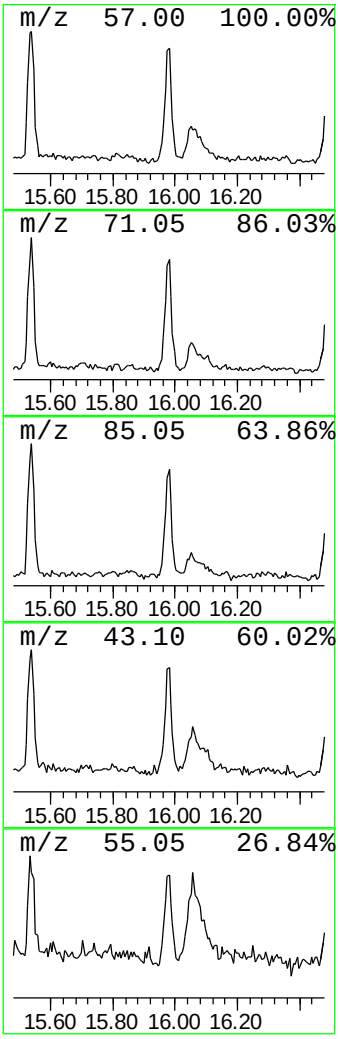
****

Peak Number 8 Nonadecane, 9-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.98	2.25 ng	125235	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	93
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Heneicosane	296	C21H44	000629-94-7	87
4	Triacontane	422	C30H62	000638-68-6	83
5	Hexacosane	366	C26H54	000630-01-3	80





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Misc :
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Instrument : BNA_F
ClientSampleId : LIED-BF003-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

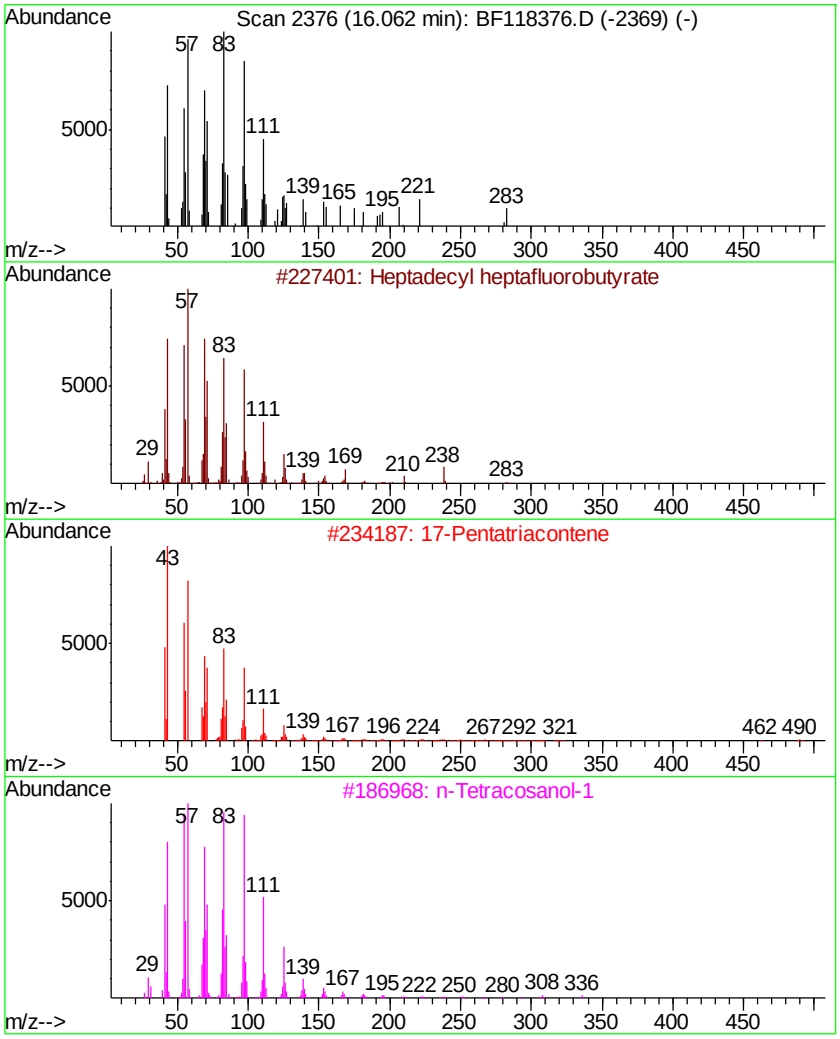
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

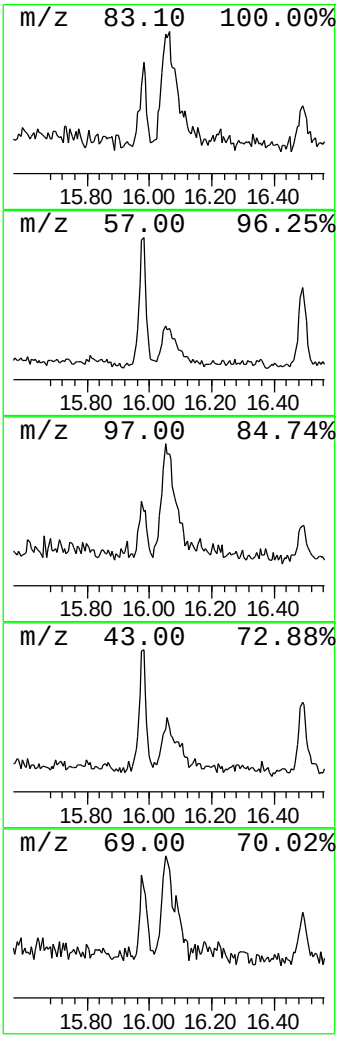
****

Peak Number 9 Heptadecyl heptafluorobutyrate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.06	2.68 ng	148792	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2	17-Pentatriacontene	491	C35H70	006971-40-0	91
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
4	1-Heptacosanol	396	C27H56O	002004-39-9	90
5	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	87





Tentatively Identified Compound (LSC) summary

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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...	5.06	19.0	ng	614688	1	6.85	647637	20.0
unknown6.63	6.63	115.7	ng	3746570	1	6.85	647637	20.0
n-Hexadecanoic acid	11.92	7.1	ng	395209	4	11.39	1113560	20.0
5-Eicosene, (E)-	13.87	12.0	ng	661879	5	14.04	1106200	20.0
Eicosane	14.81	2.7	ng	150380	6	15.54	1111350	20.0
Nonadecane, 9-met...	15.98	2.3	ng	125235	6	15.54	1111350	20.0
Heptadecyl heptaf...	16.06	2.7	ng	148792	6	15.54	1111350	20.0