LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070518\
Data File : BF107127.D
Acq On : 5 Jul 2018 15:24
Operator : JU/SJ
Sample : J3853-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B2

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-BF061918.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	5.189	481	485	499	rBB	141689	165034	12.35%	1.416%
2	5.595	550	554	569	rBV	1210435	1143115	85.55%	9.811%
3	6.595	720	724	742	rBV	1045907	1171676	87.69%	10.056%
4	6.731	742	747	750	rBV	1301901	1194657	89.41%	10.253%
5	6.948	781	784	788	rBV	402222	332656	24.90%	2.855%
6	7.107	807	811	814	rBV	1075692	960389	71.87%	8.243%
7	7.519	875	881	884	rBV	716648	753465	56.39%	6.467%
8	8.230	998	1002	1016	rBV	416179	424088	31.74%	3.640%
9	9.307	1180	1185	1188	rBV	1500216	1336195	100.00%	11.468%
10	9.695	1248	1251	1261	rBB	197763	186174	13.93%	1.598%
11	9.995	1298	1302	1309	rVB	499979	462184	34.59%	3.967%
12	10.789	1433	1437	1447	rBV	877395	801429	59.98%	6.878%
13	11.489	1552	1556	1563	rBV	469759	410789	30.74%	3.526%
14	11.689	1587	1590	1594	rBV	16746	19322	1.45%	0.166%
15	11.971	1622	1638	1640	rBV8	9960	37392	2.80%	0.321%
16	12.236	1680	1683	1687	rVB2	25566	20283	1.52%	0.174%
17	12.760	1765	1772	1773	rBV7	12760	28237	2.11%	0.242%
18	12.854	1775	1788	1789	rBV9	38288	121830	9.12%	1.046%
19	13.071	1821	1825	1828	rVB	1165780	1037538	77.65%	8.905%
20	13.948	1972	1974	1977	rVB	55755	44779	3.35%	0.384%
21	14.142	2004	2007	2012	rBV	383000	374923	28.06%	3.218%
22	14.977	2147	2149	2154	rVB	154191	157519	11.79%	1.352%
23	15.689	2267	2270	2279	rVB	325067	467667	35.00%	4.014%

Sum of corrected areas: 11651341

LSC Report - Integrated Chromatogram

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Misc :
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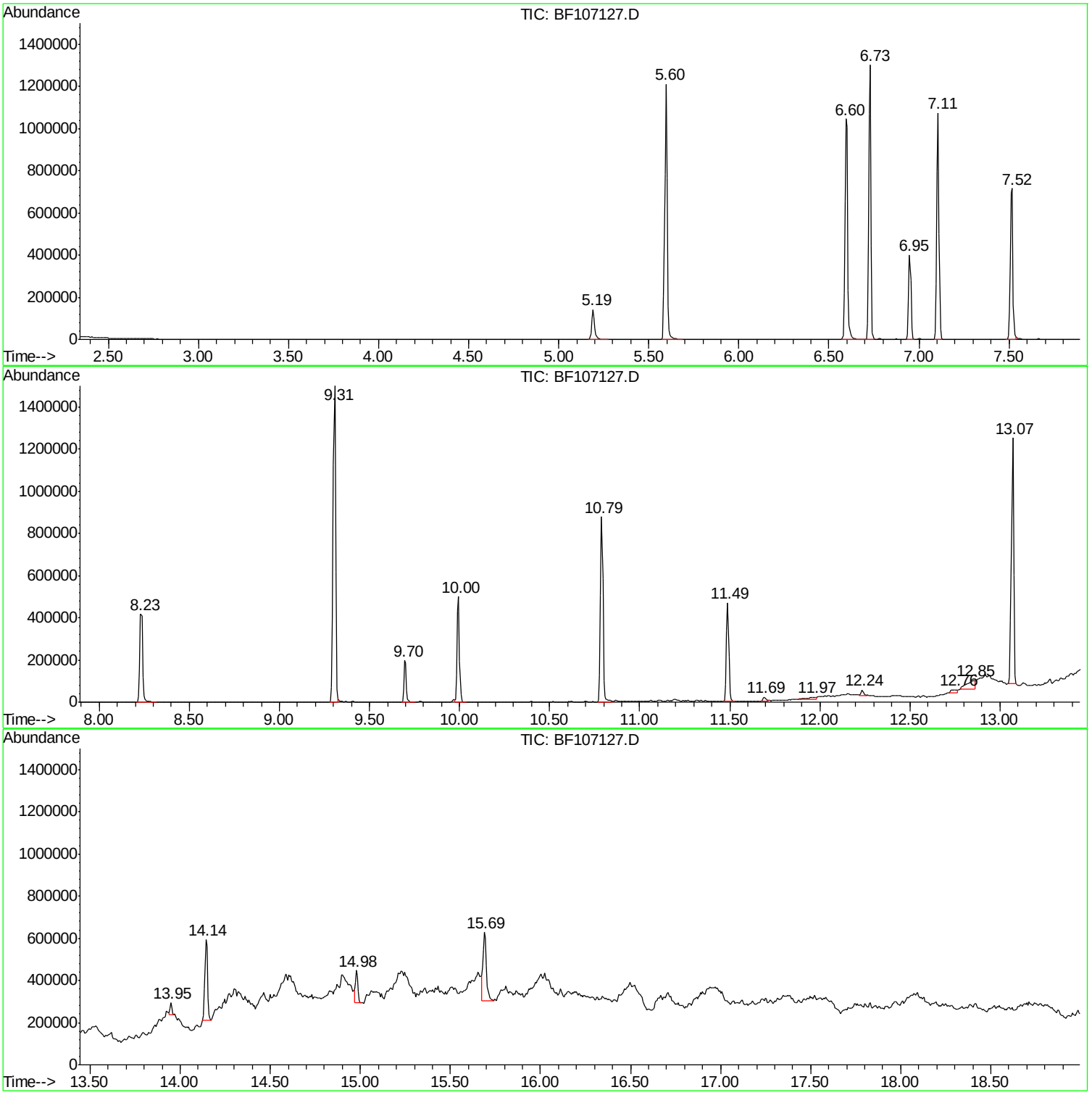
Instrument : BNA_F
ClientSampleId : B2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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\BF070518\
Data File : BF107127.D
Acq On : 5 Jul 2018 15:24
Operator : JU/SJ
Sample : J3853-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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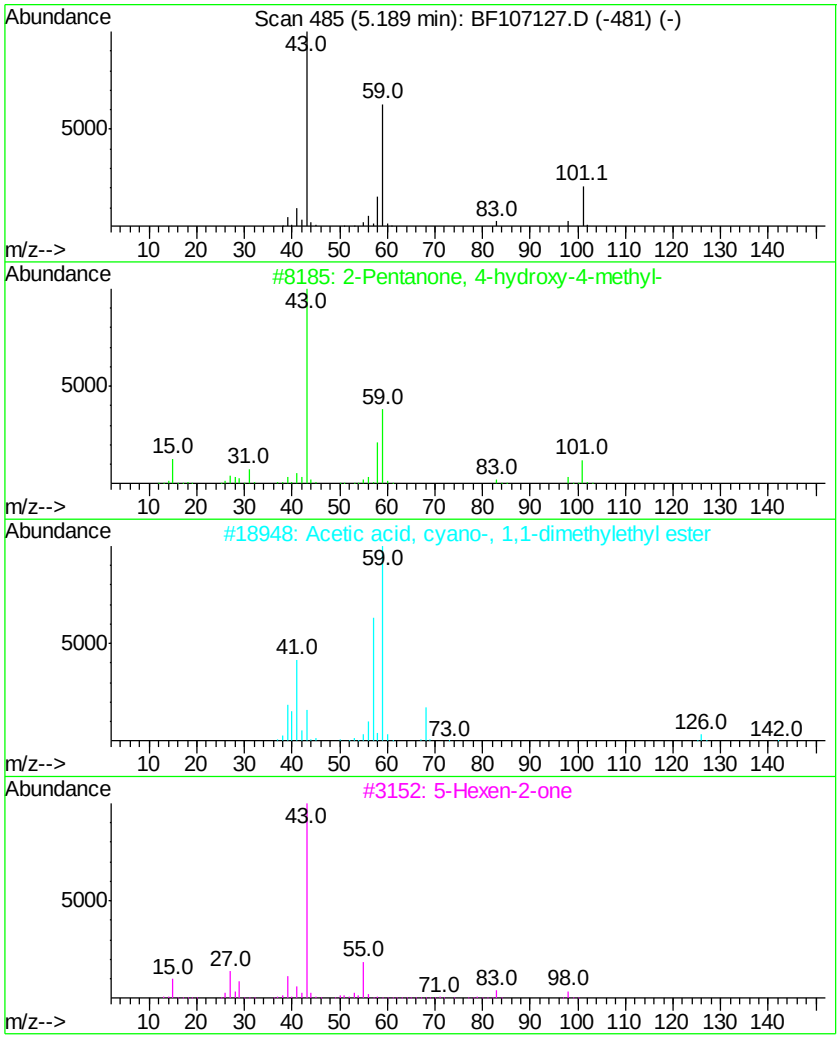
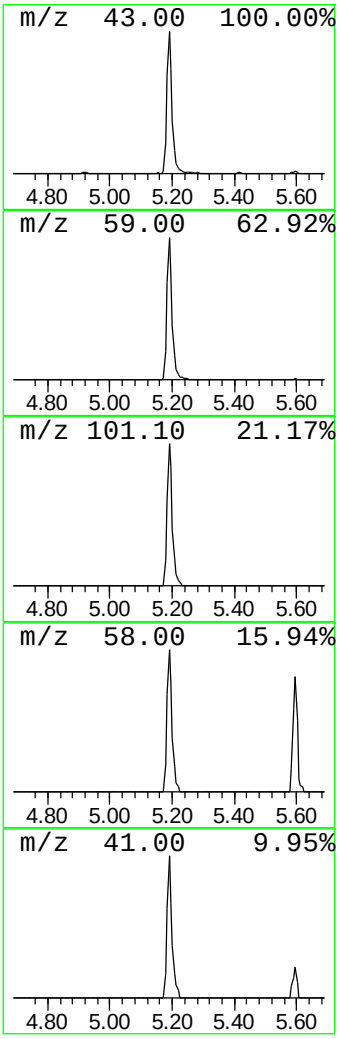
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	9.92 ng	165034	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Sample : J3853-03
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Instrument : BNA_F
ClientSampleId : B2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
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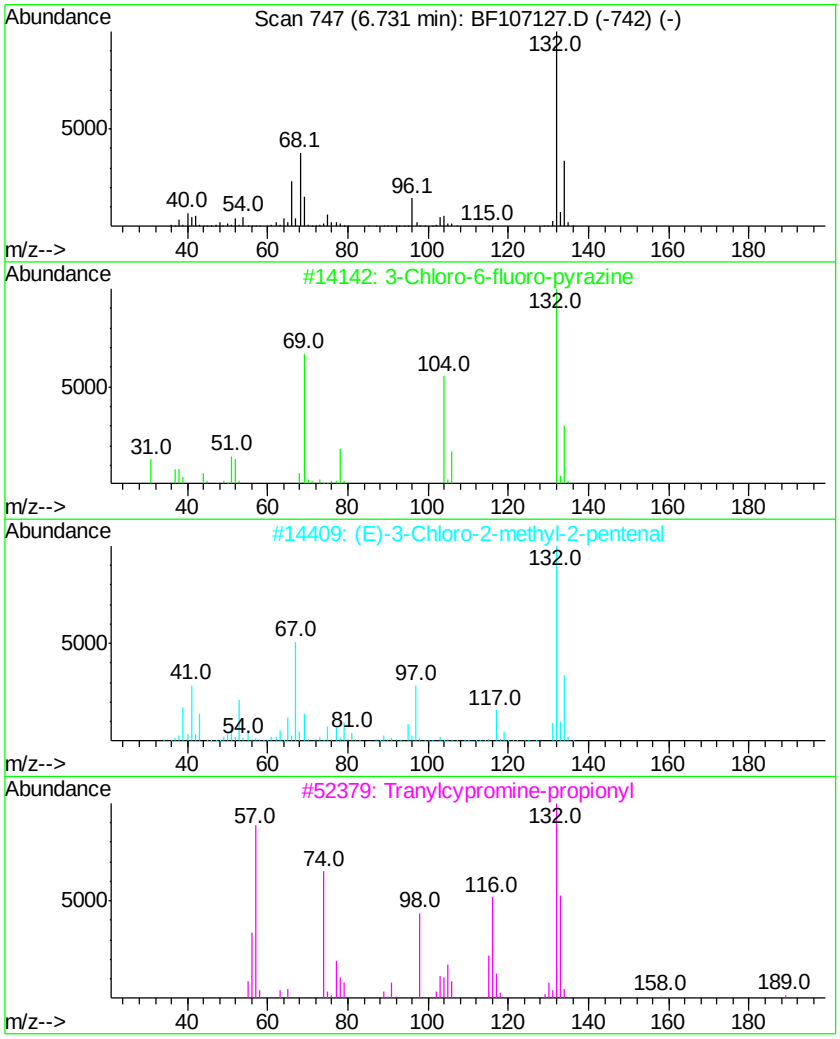
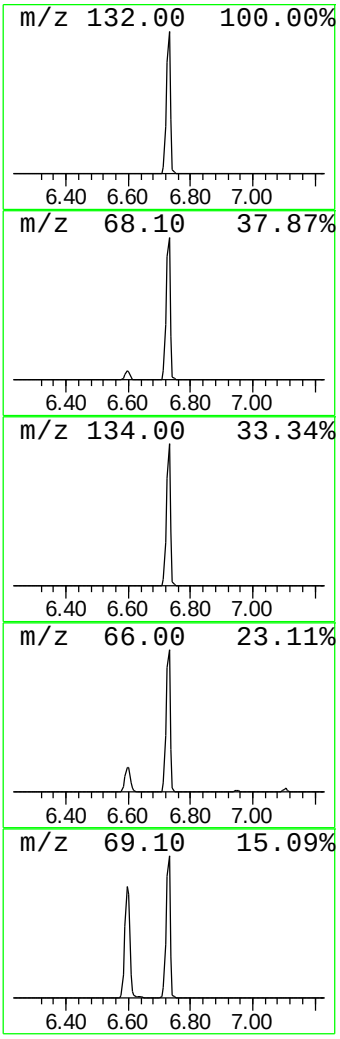
Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	71.83 ng	1194660	1,4-Dichlorobenzene-d4	6.95

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	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10





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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
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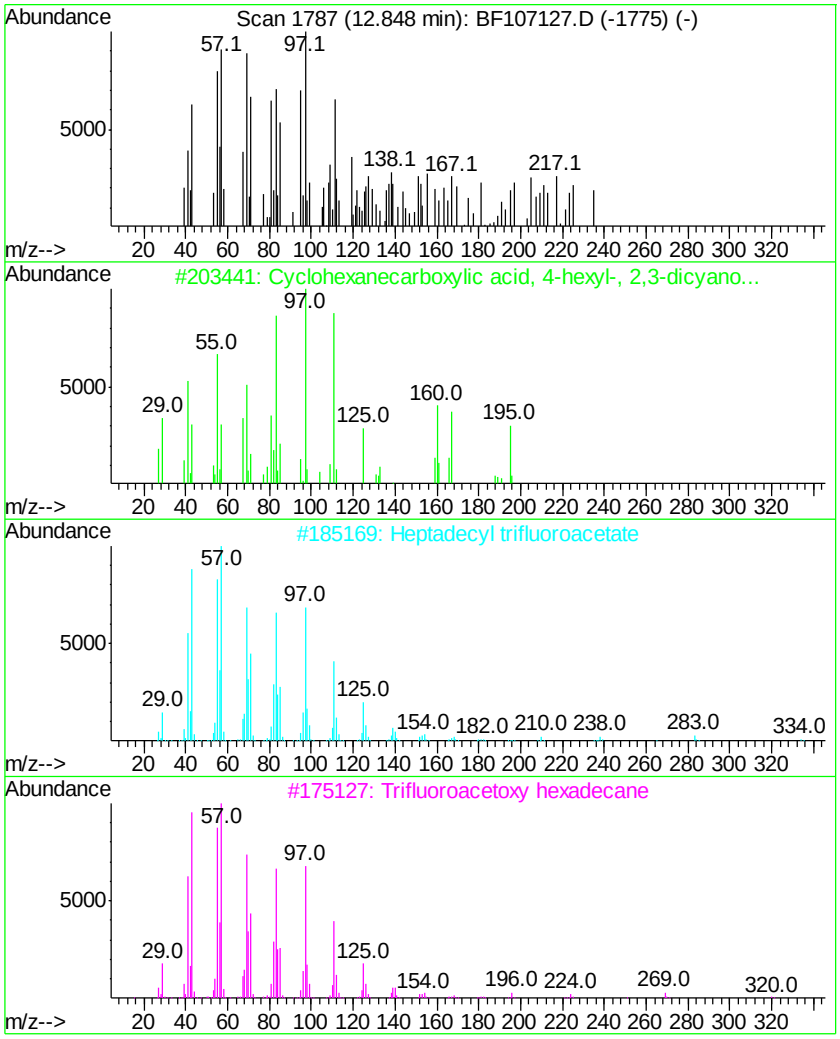
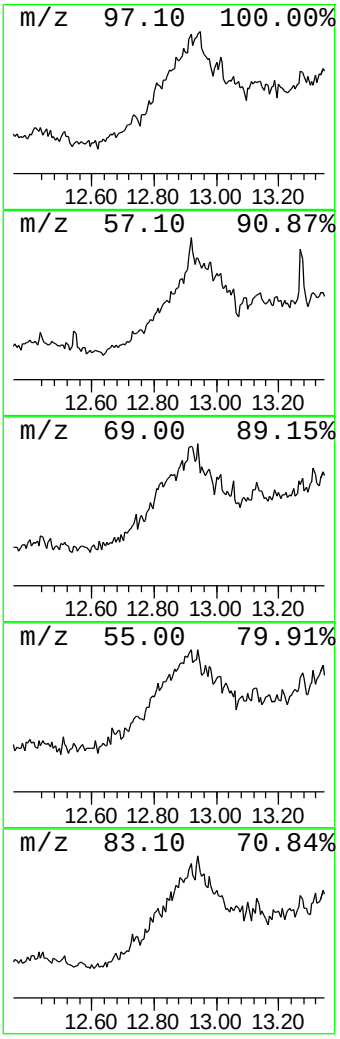
Peak Number 4 unknown12.85 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.85	6.50 ng	121830	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanecarboxylic acid, 4-he...	382	C23H30N2O3	133856-88-9	43
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	41
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	38
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	38
5	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	38





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
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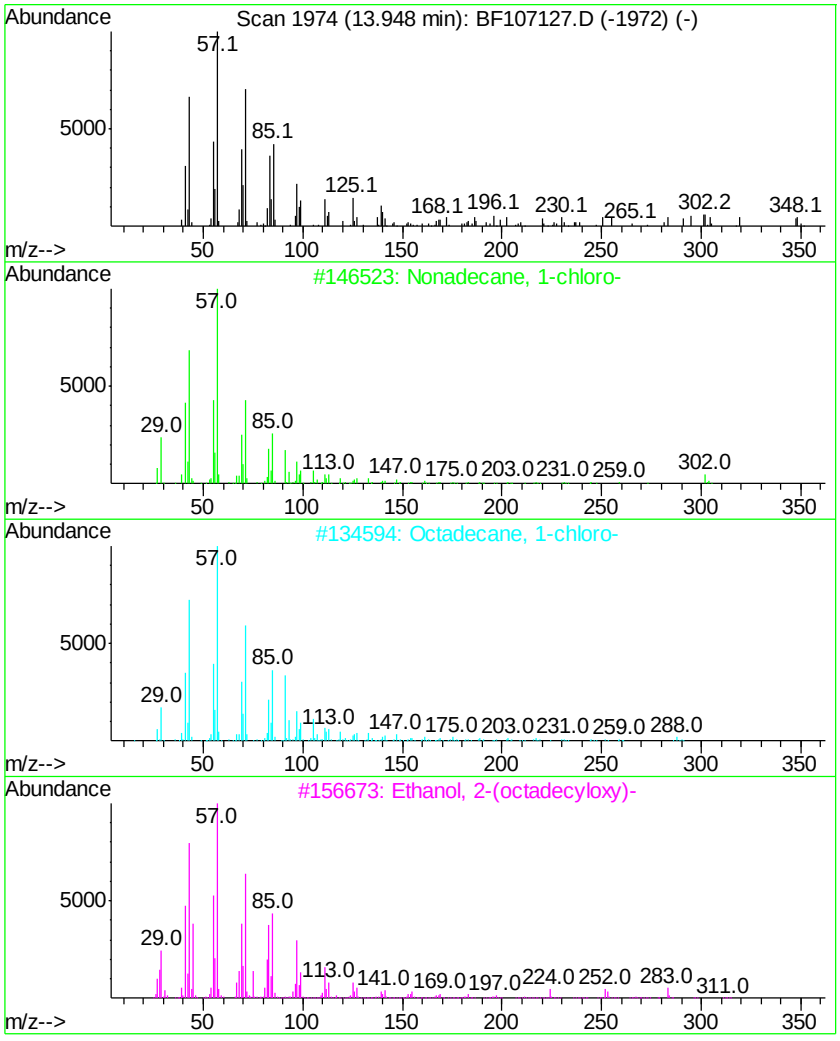
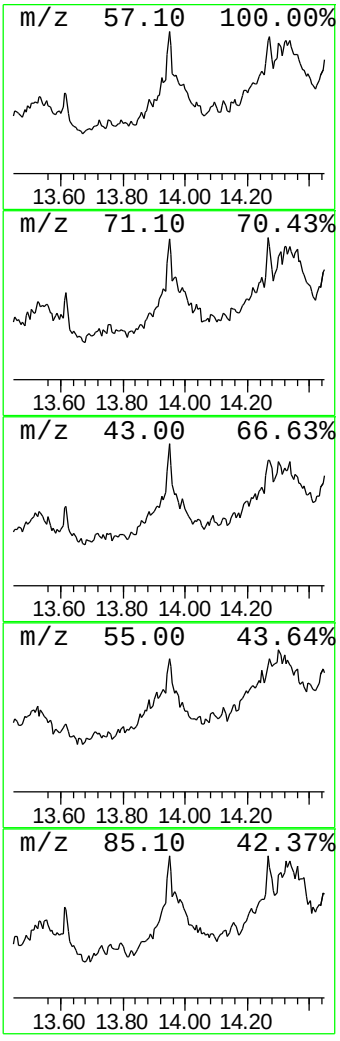
Peak Number 5 Nonadecane, 1-chloro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	2.39 ng	44779	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	90
2	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	64
3	Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	64
4	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	64
5	Hexadecane	226	C16H34	000544-76-3	60





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Instrument : BNA_F
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TIC Integration Parameters: LSCINT.P

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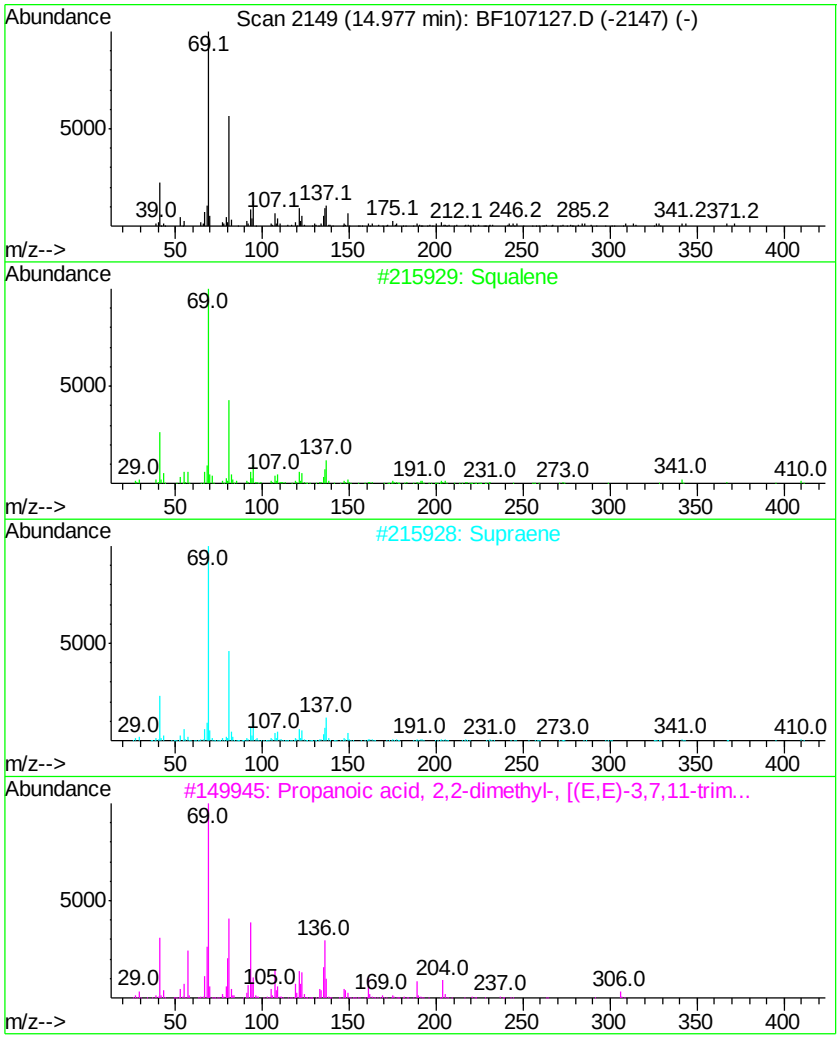
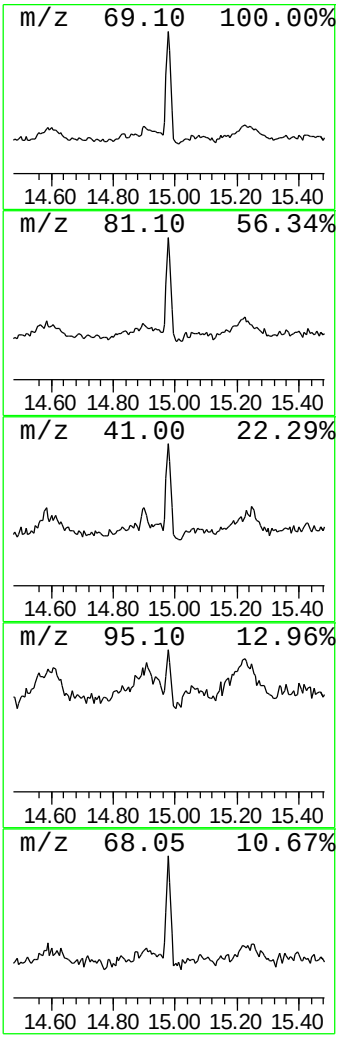
Peak Number 6 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	6.74 ng	157519	Perylene-d12	15.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	86
2	Supraene	410	C30H50	007683-64-9	83
3	Propanoic acid, 2,2-dimethyl-, [...	306	C20H34O2	1000164-38-8	64
4	Trideca-1,3,7,11-tetraene-1,1-di...	268	C18H24N2	1000159-88-9	59
5	2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	50





Tentatively Identified Compound (LSC) summary

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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...	5.19	9.9	ng	165034	1	6.95	332656	20.0
unknown6.73	6.73	71.8	ng	1194660	1	6.95	332656	20.0
unknown12.85	12.85	6.5	ng	121830	5	14.14	374923	20.0
Nonadecane, 1-chl...	13.95	2.4	ng	44779	5	14.14	374923	20.0
Squalene	14.98	6.7	ng	157519	6	15.69	467667	20.0