LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112519\
Data File : BF117988.D
Acq On : 26 Nov 2019 1:43
Operator : JU
Sample : K5840-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NE-03

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-BF111319.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	2.181	11	16	24	rVB	658168	828753	20.37%	2.466%
2	5.104	504	513	522	rBV	622244	783883	19.27%	2.332%
3	5.504	576	581	584	rBV	3188729	3156505	77.59%	9.391%
4	6.516	747	753	766	rBV	2917294	3236628	79.56%	9.629%
5	6.657	772	777	780	rBV	3623584	3511442	86.31%	10.446%
6	6.886	813	816	820	rBV	1275704	1055037	25.93%	3.139%
7	7.045	839	843	847	rBV	3155469	2812608	69.13%	8.367%
8	7.451	907	912	915	rBV	1906087	1895843	46.60%	5.640%
9	8.175	1031	1035	1039	rBV	1697089	1372655	33.74%	4.084%
10	9.257	1214	1219	1222	rBV	4731893	4068374	100.00%	12.103%
11	9.645	1282	1285	1289	rVB	381155	313365	7.70%	0.932%
12	9.939	1331	1335	1338	rBV	1691774	1334823	32.81%	3.971%
13	10.727	1465	1469	1473	rBV	2230180	2077595	51.07%	6.181%
14	11.433	1585	1589	1592	rBV	1516713	1364137	33.53%	4.058%
15	11.951	1674	1677	1690	rVB	215357	213085	5.24%	0.634%
16	12.739	1808	1811	1817	rBV2	61476	64060	1.57%	0.191%
17	13.021	1854	1859	1862	rBV	3357353	2811523	69.11%	8.364%
18	13.921	2008	2012	2022	rVB2	196234	369989	9.09%	1.101%
19	14.080	2035	2039	2042	rBV	888126	838743	20.62%	2.495%
20	14.186	2050	2057	2063	rBV2	56893	179126	4.40%	0.533%
21	14.545	2115	2118	2121	rBV	43604	46790	1.15%	0.139%
22	14.715	2143	2147	2149	rBV5	28467	46065	1.13%	0.137%
23	14.939	2181	2185	2192	rVB	196680	245254	6.03%	0.730%
24	15.204	2227	2230	2236	rBV2	75540	138492	3.40%	0.412%
25	15.574	2288	2293	2297	rBV	651865	793277	19.50%	2.360%
26	16.056	2372	2375	2382	rVB2	36072	55745	1.37%	0.166%

Sum of corrected areas: 33613797

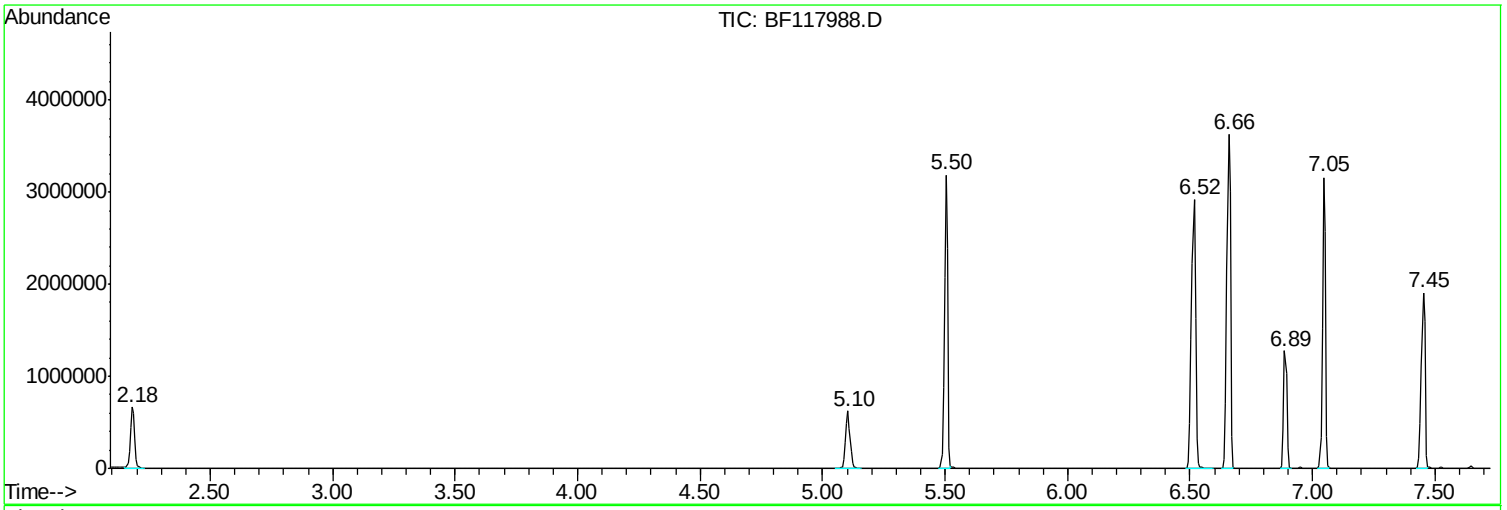
LSC Report - Integrated Chromatogram

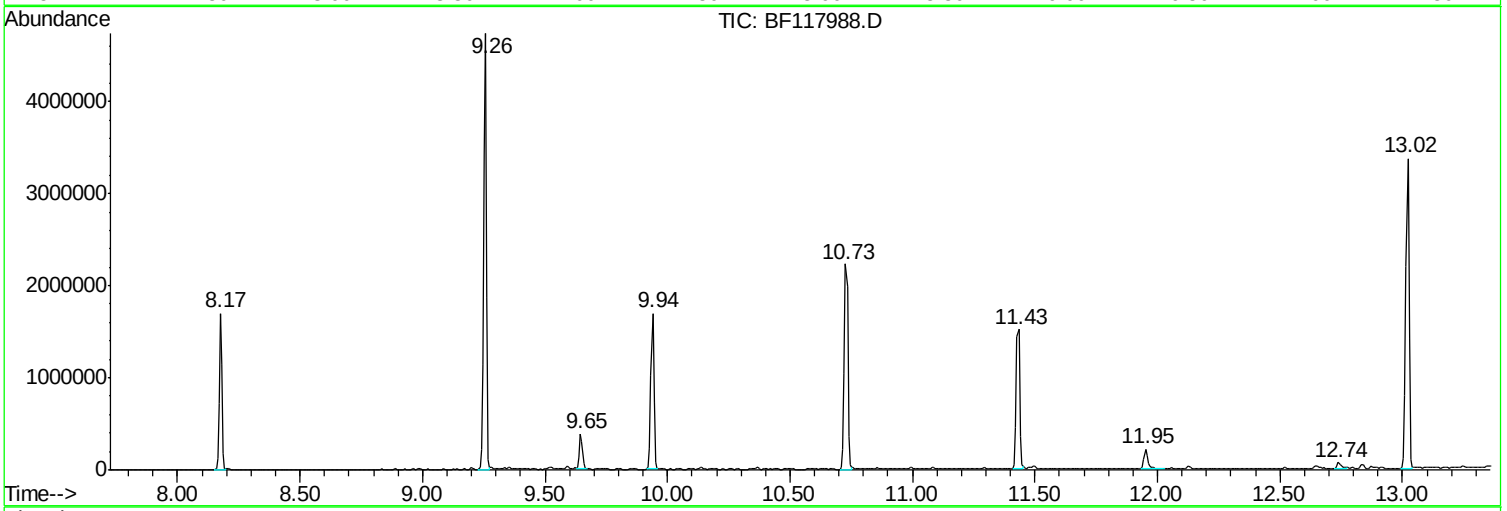
Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112519\
Data File : BF117988.D
Acq On : 26 Nov 2019 1:43
Operator : JU
Sample : K5840-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

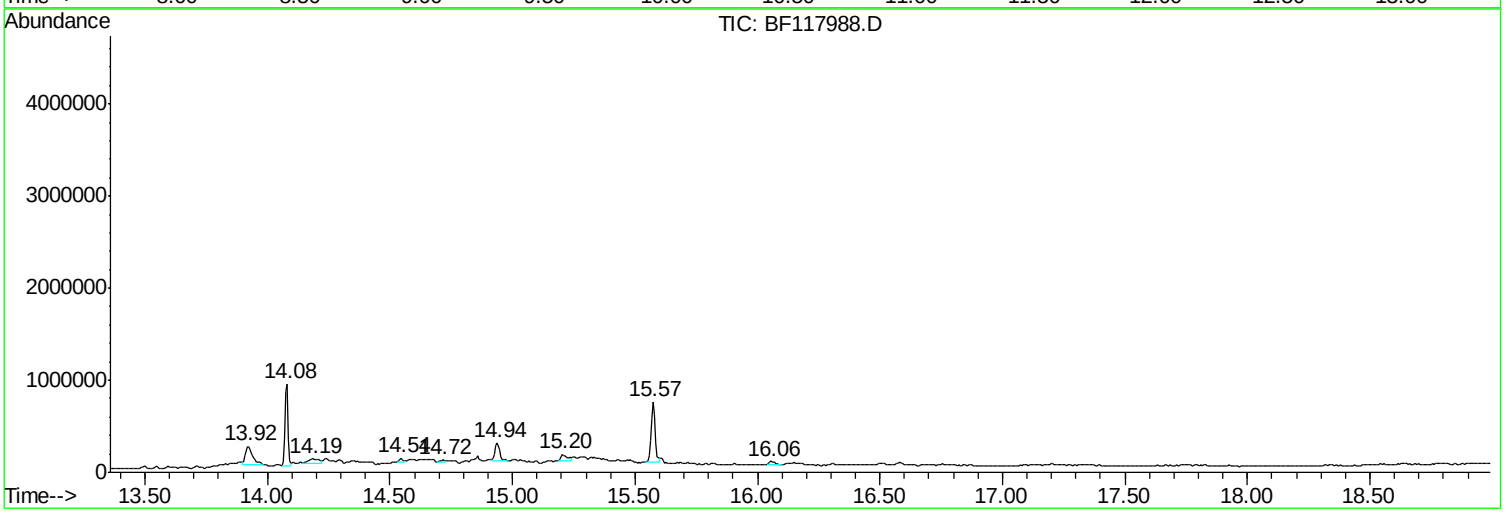
Instrument :
BNA_F
ClientSampleId :
PHIPPS-BH-NE-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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\BF112519\
Data File : BF117988.D
Acq On : 26 Nov 2019 1:43
Operator : JU
Sample : K5840-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NE-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

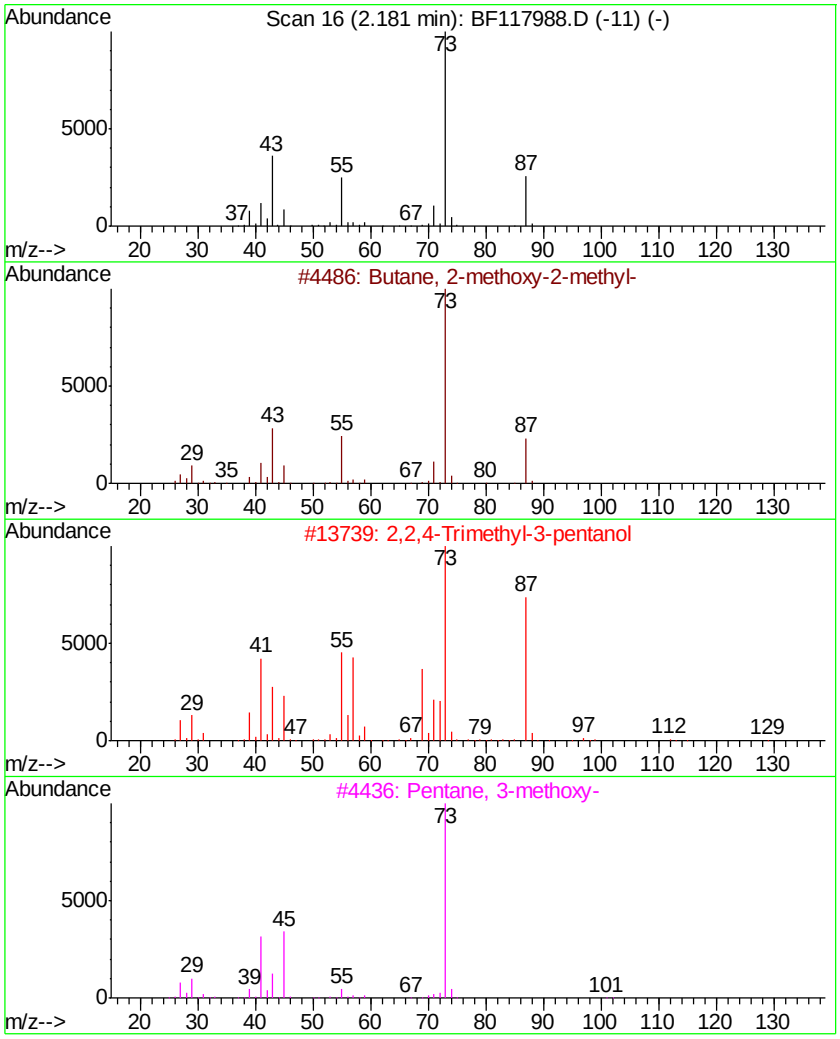
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

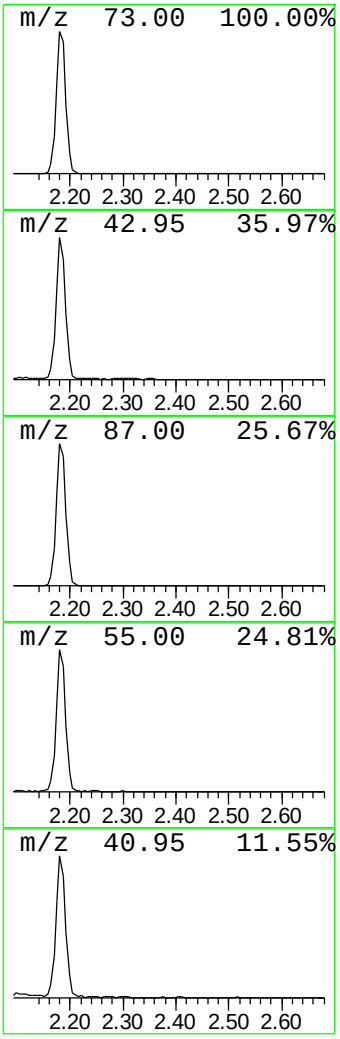
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	15.71 ng	828753	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112519\
Data File : BF117988.D
Acq On : 26 Nov 2019 1:43
Operator : JU
Sample : K5840-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NE-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

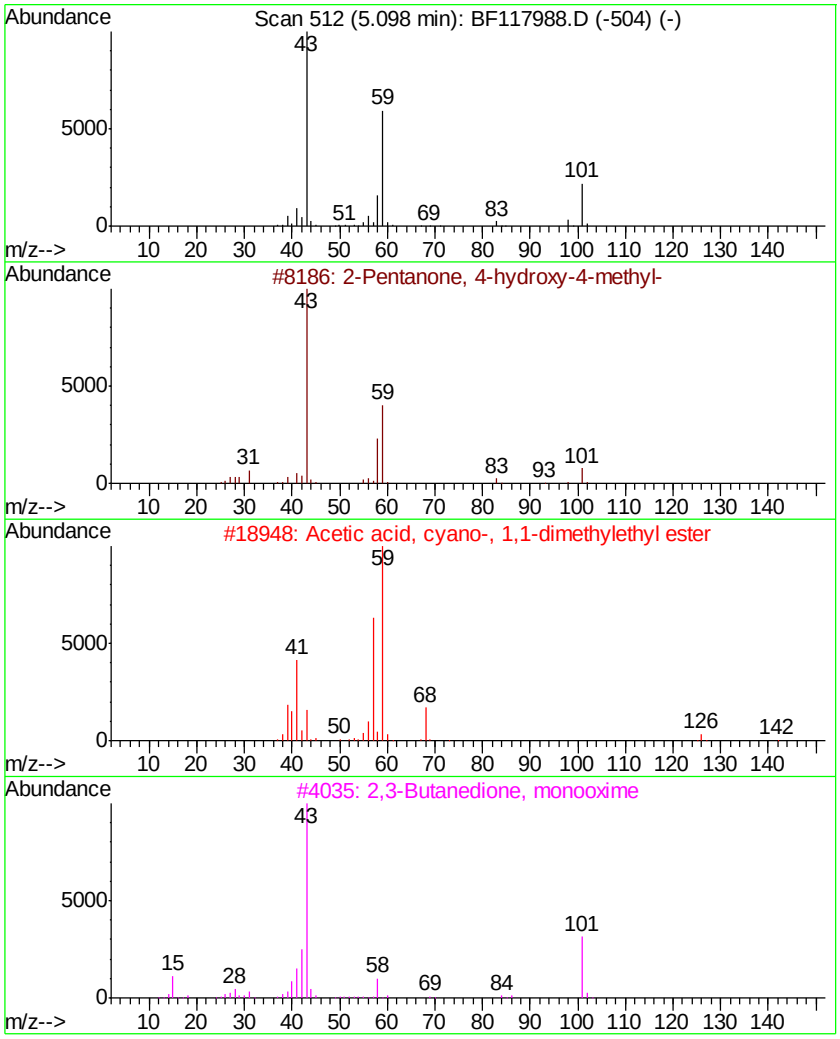
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

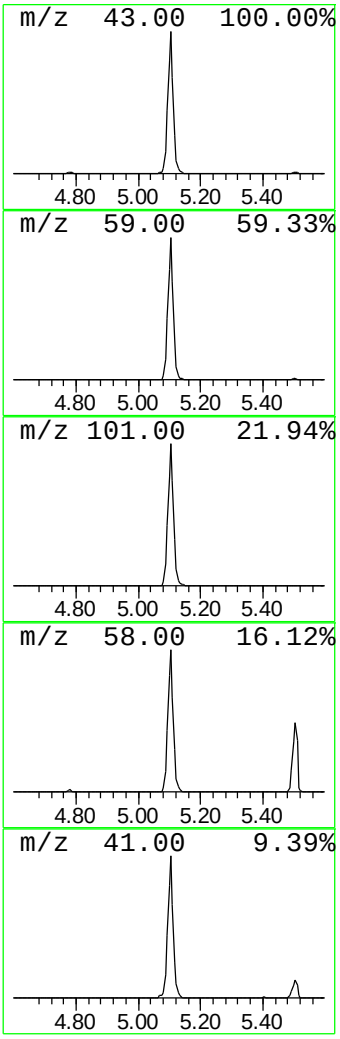
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	14.86 ng	783883	1,4-Dichlorobenzene-d4	6.89

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	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Data File : BF117988.D
Acq On : 26 Nov 2019 1:43
Operator : JU
Sample : K5840-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NE-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

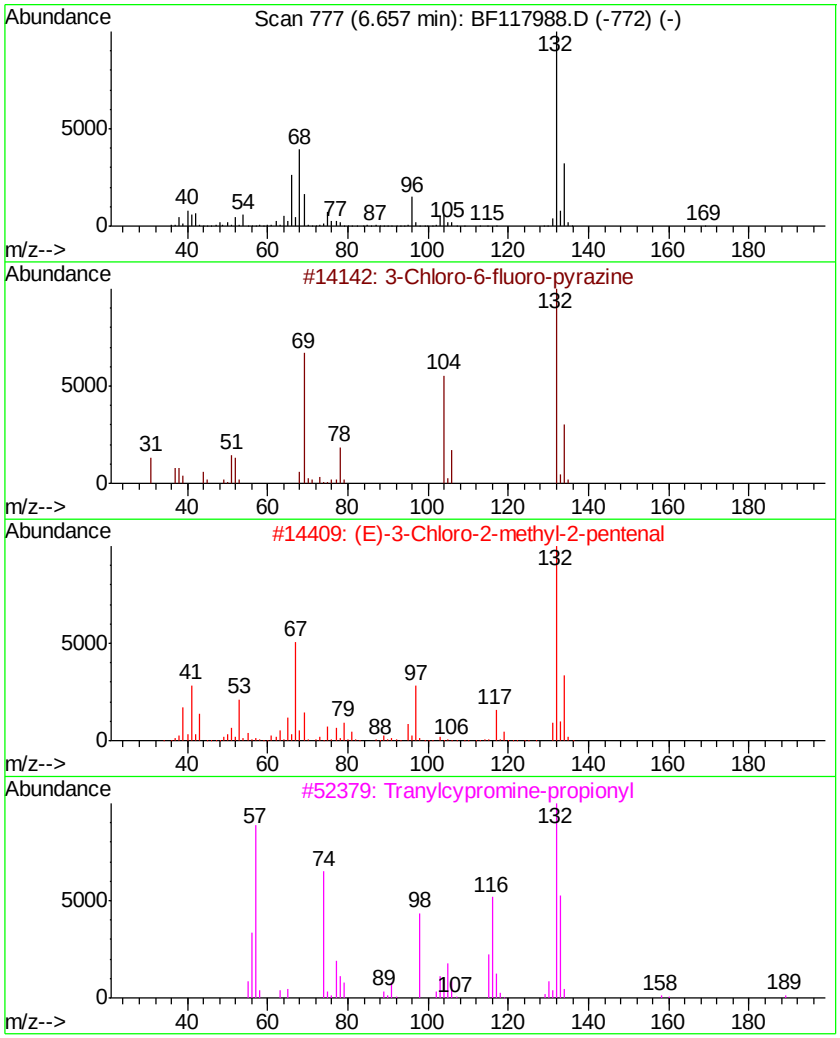
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

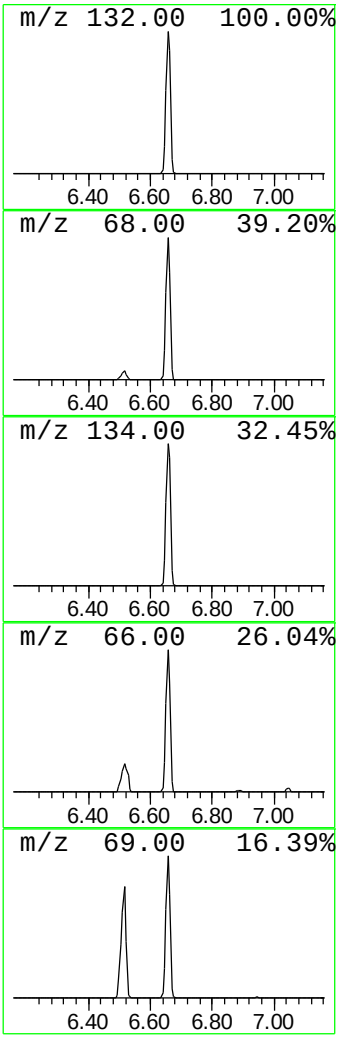
****

Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	66.57 ng	3511440	1,4-Dichlorobenzene-d4	6.89

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	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112519\
Data File : BF117988.D
Acq On : 26 Nov 2019 1:43
Operator : JU
Sample : K5840-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NE-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

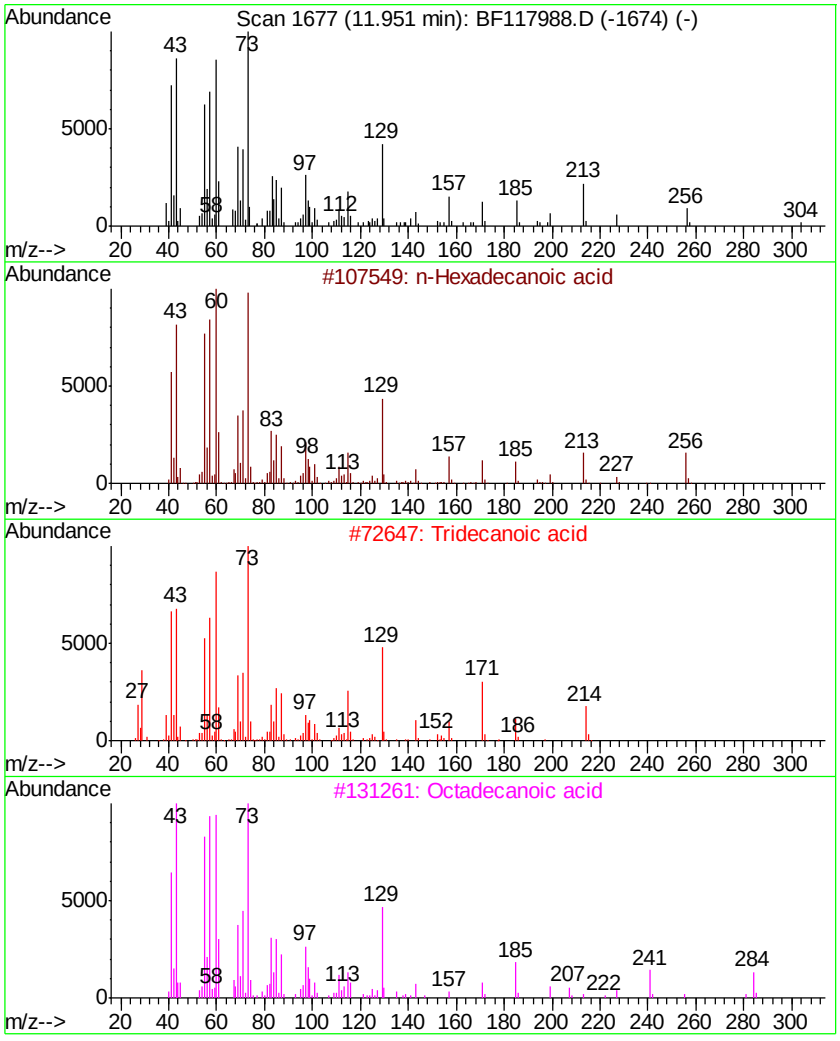
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

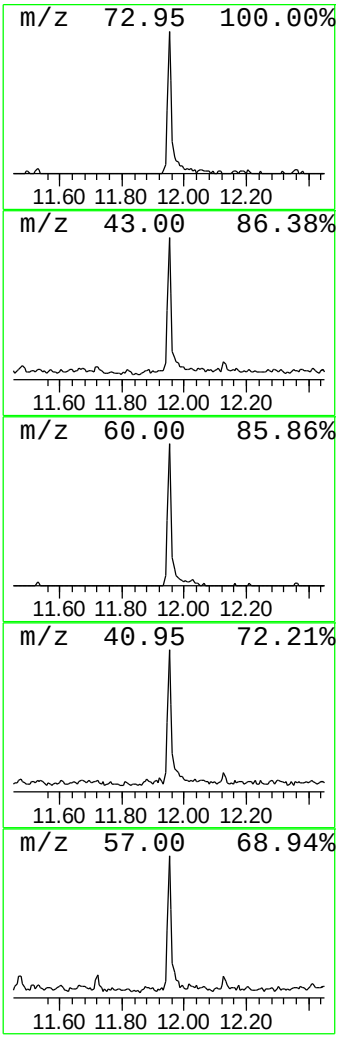
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	3.12 ng	213085	Phenanthrene-d10	11.43

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	Octadecanoic acid	284	C18H36O2	000057-11-4	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	80





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112519\
Data File : BF117988.D
Acq On : 26 Nov 2019 1:43
Operator : JU
Sample : K5840-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NE-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

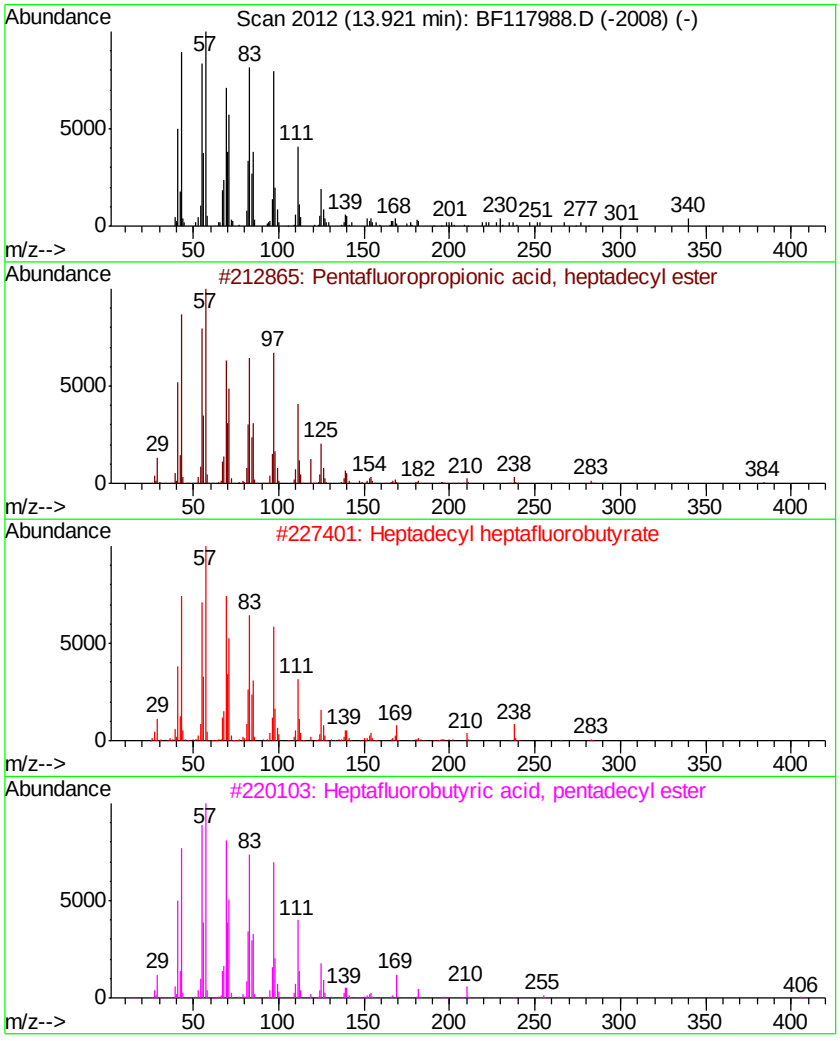
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

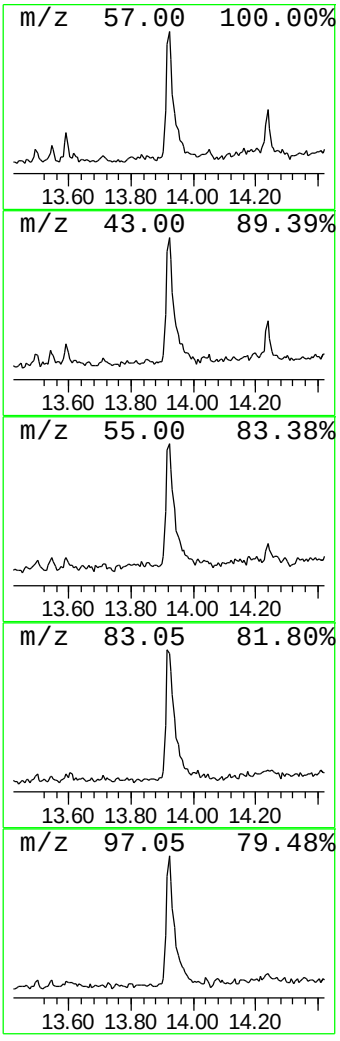
****

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	8.82 ng	369989	Chrysene-d12	14.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	95
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112519\
Data File : BF117988.D
Acq On : 26 Nov 2019 1:43
Operator : JU
Sample : K5840-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NE-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

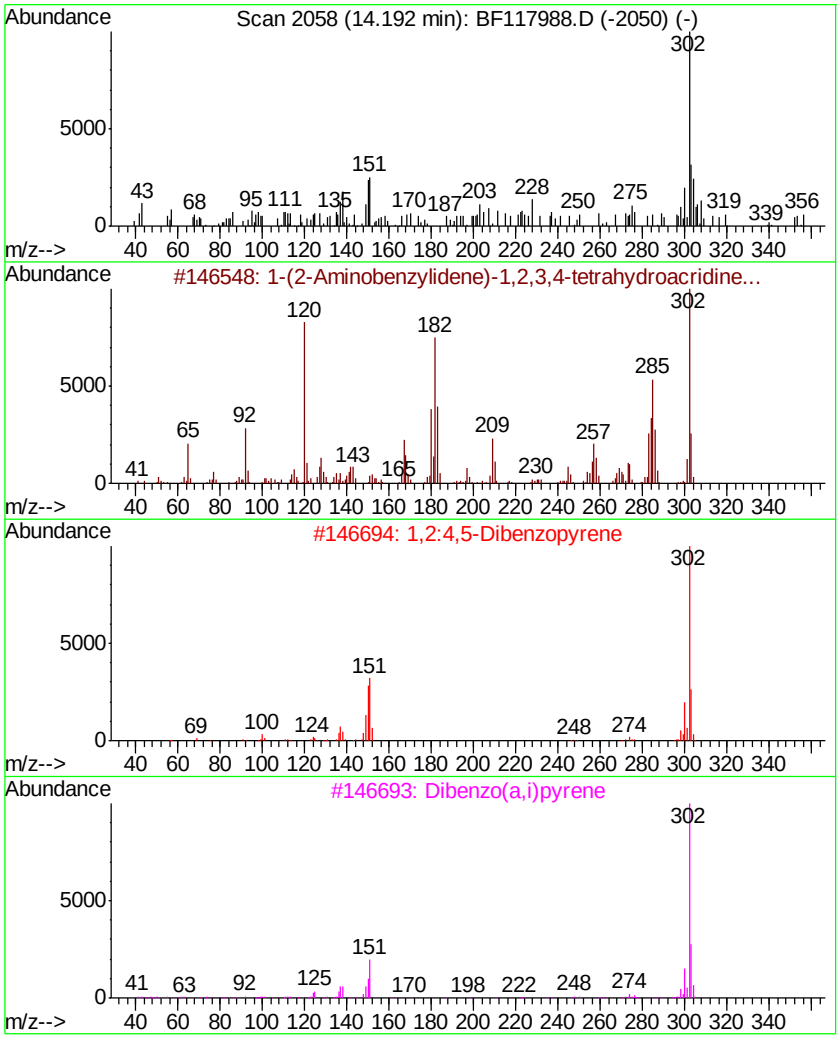
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

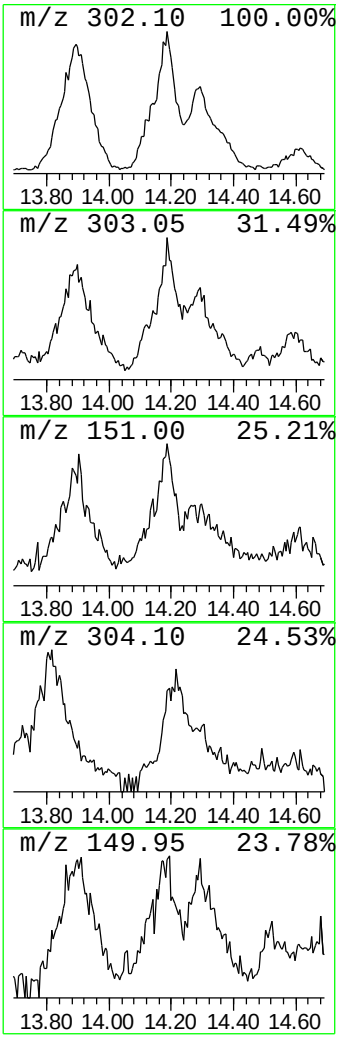
****

Peak Number 7 1-(2-Aminobenzylidene)-1,2,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.19	4.27 ng	179126	Chrysene-d12	14.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(2-Aminobenzylidene)-1,2,3,4-t...	302	C20H18N2O	1000110-40-2	90
2	1,2:4,5-Dibenzopyrene	302	C24H14	000192-65-4	70
3	Dibenzo(a,i)pyrene	302	C24H14	000189-55-9	70
4	3,4:8,9-Dibenzopyrene	302	C24H14	000189-64-0	64
5	Coronene, 1,2-dihydro-	302	C24H14	107716-56-3	53





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112519\
Data File : BF117988.D
Acq On : 26 Nov 2019 1:43
Operator : JU
Sample : K5840-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NE-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

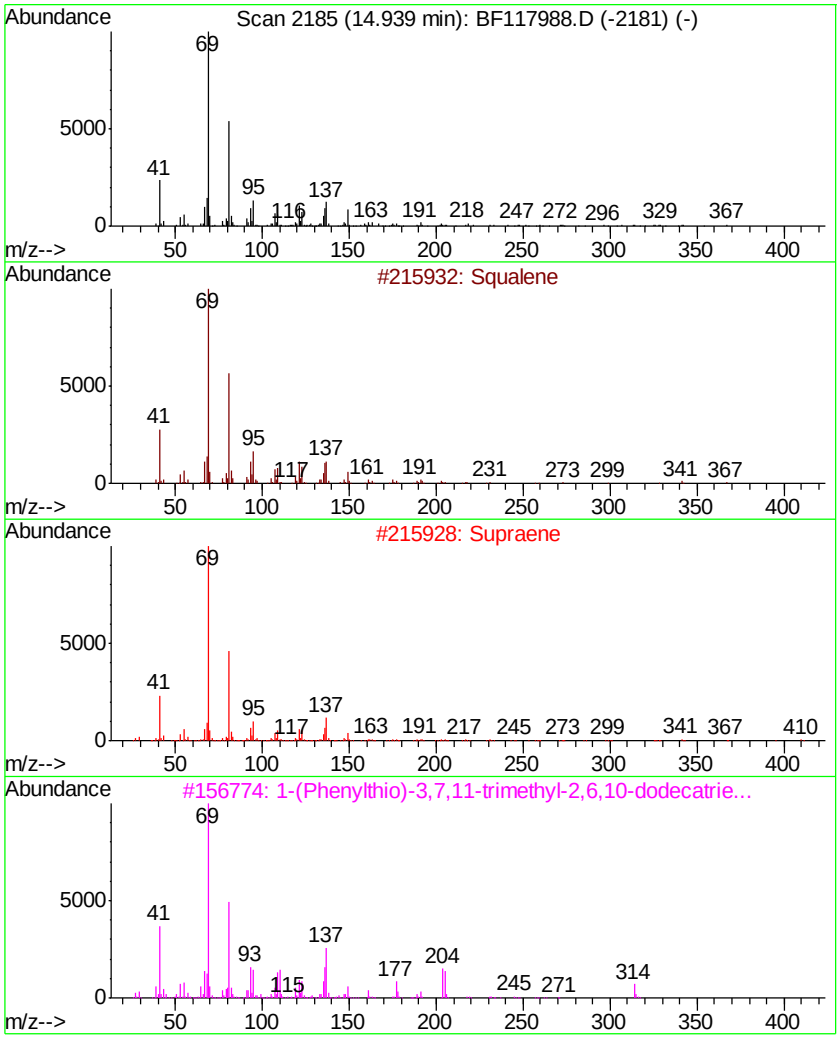
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

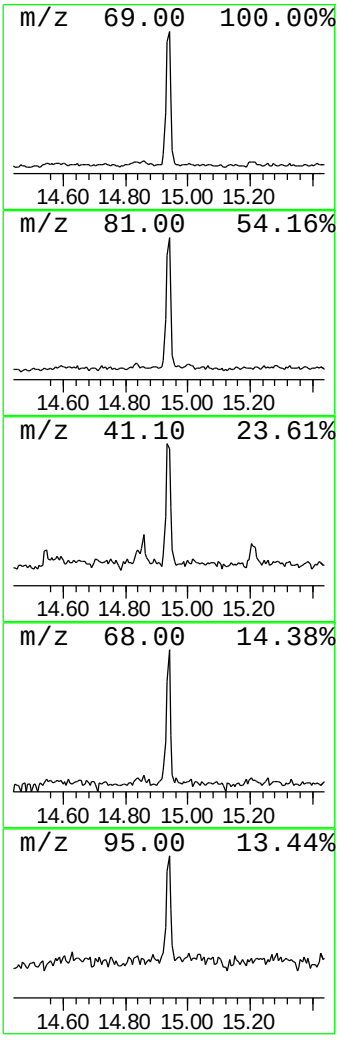
****

Peak Number 8 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	6.18 ng	245254	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	1-(Phenylthio)-3,7,11-trimethyl-...	314	C21H30S	028413-57-2	90
4	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
5	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112519\
Data File : BF117988.D
Acq On : 26 Nov 2019 1:43
Operator : JU
Sample : K5840-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NE-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

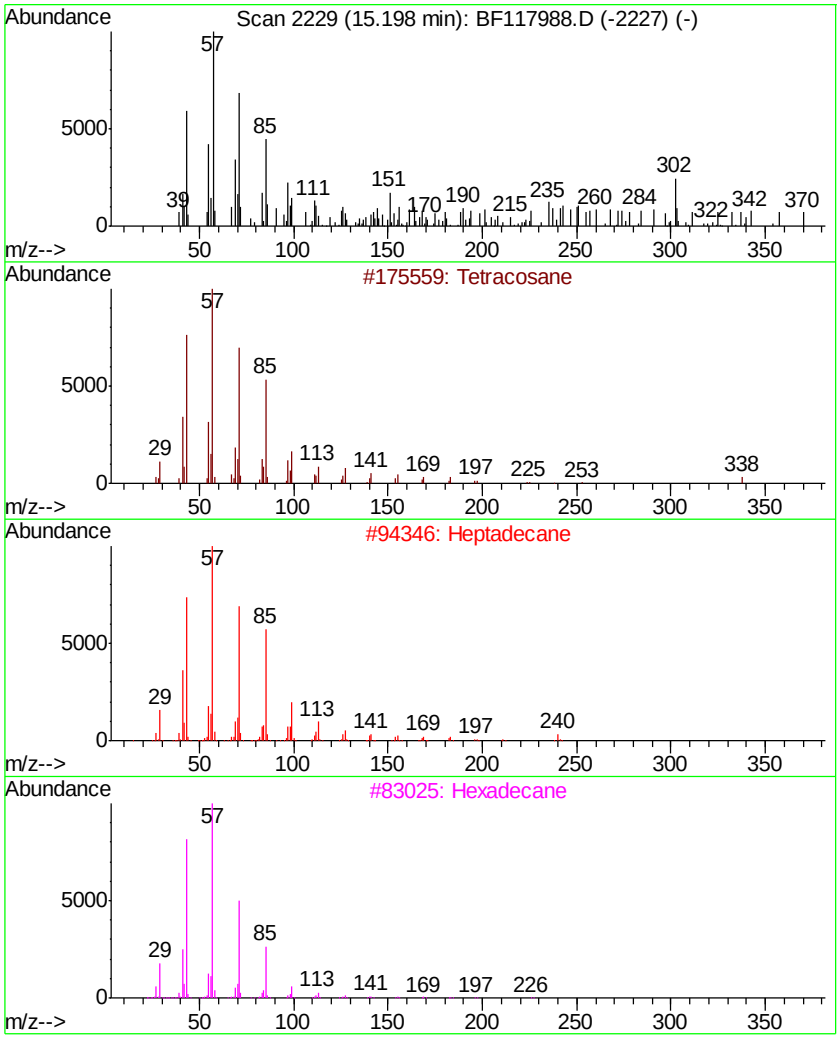
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

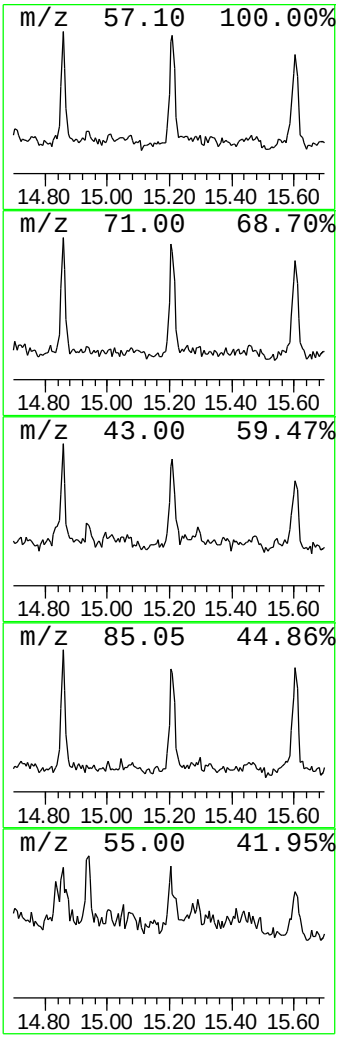
****

Peak Number 9 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.20	3.49 ng	138492	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	93
2	Heptadecane	240	C17H36	000629-78-7	91
3	Hexadecane	226	C16H34	000544-76-3	83
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	78
5	Nonadecane	268	C19H40	000629-92-5	78





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112519\
Data File : BF117988.D
Acq On : 26 Nov 2019 1:43
Operator : JU
Sample : K5840-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NE-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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...	2.18	15.7	ng	828753	1	6.89	1055040	20.0
2-Pentanone, 4-hy...	5.10	14.9	ng	783883	1	6.89	1055040	20.0
unknown6.66	6.66	66.6	ng	3511440	1	6.89	1055040	20.0
n-Hexadecanoic acid	11.95	3.1	ng	213085	4	11.43	1364140	20.0
Pentafluoropropio...	13.92	8.8	ng	369989	5	14.08	838743	20.0
1-(2-Aminobenzyli...	14.19	4.3	ng	179126	5	14.08	838743	20.0
Squalene	14.94	6.2	ng	245254	6	15.57	793277	20.0
Tetracosane	15.20	3.5	ng	138492	6	15.57	793277	20.0