LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117707.D
Acq On : 7 Nov 2019 16:26
Operator : JU
Sample : K5710-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP- 32-S

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-BF110619.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	2.246	19	27	32	rBV	1446517	1915942	24.40%	2.583%
2	5.157	512	522	529	rVB	1183828	1519621	19.35%	2.049%
3	5.551	583	589	592	rBV	6333296	6668284	84.91%	8.991%
4	6.551	753	759	763	rBV	6656192	7145885	90.99%	9.635%
5	6.704	780	785	788	rBV	6928480	7128416	90.77%	9.612%
6	6.934	820	824	827	rBV	2486983	1928268	24.55%	2.600%
7	7.092	847	851	854	rVB	6583145	5576495	71.01%	7.519%
8	7.492	914	919	922	rBV	4505569	4417899	56.25%	5.957%
9	8.222	1038	1043	1046	rBV	2914629	2548037	32.45%	3.436%
10	9.298	1221	1226	1229	rBV	8481324	7853399	100.00%	10.589%
11	9.686	1289	1292	1296	rVB	1477472	1219605	15.53%	1.644%
12	9.980	1337	1342	1345	rBV	3418027	2858886	36.40%	3.855%
13	10.769	1471	1476	1479	rBV	5494211	4806105	61.20%	6.480%
14	11.469	1591	1595	1598	rBV	3157313	2772779	35.31%	3.739%
15	11.539	1602	1607	1610	rVB3	214720	205350	2.61%	0.277%
16	11.998	1678	1685	1691	rBV2	838025	988883	12.59%	1.333%
17	12.686	1799	1802	1807	rBV	124371	137590	1.75%	0.186%
18	12.780	1815	1818	1825	rBV	273941	316583	4.03%	0.427%
19	12.916	1838	1841	1843	rBV	171775	136769	1.74%	0.184%
20	13.063	1861	1866	1869	rBV	7461517	6508298	82.87%	8.776%
21	13.957	2014	2018	2027	rBV	779632	825548	10.51%	1.113%
22	14.115	2041	2045	2048	rBV	2339493	2100573	26.75%	2.832%
23	14.280	2071	2073	2079	rVB	102758	107117	1.36%	0.144%
24	14.592	2123	2126	2130	rVB	188335	179887	2.29%	0.243%
25	14.909	2177	2180	2184	rBV	163875	187465	2.39%	0.253%
26	14.992	2191	2194	2200	rVB	255917	265097	3.38%	0.357%
27	15.180	2222	2226	2229	rBV	122779	206570	2.63%	0.279%
28	15.268	2237	2241	2251	rVB2	195385	320765	4.08%	0.433%
29	15.492	2276	2279	2285	rBV	116308	139805	1.78%	0.189%
30	15.557	2287	2290	2294	rVB	138552	169484	2.16%	0.229%
31	15.627	2297	2302	2306	rVV2	1853389	2293353	29.20%	3.092%
32	15.674	2306	2310	2316	rVB2	181342	284062	3.62%	0.383%
33	16.139	2385	2389	2393	rBV	109110	177898	2.27%	0.240%
34	16.186	2394	2397	2407	rVB8	117491	252802	3.22%	0.341%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117707.D
Acq On : 7 Nov 2019 16:26
Operator : JU
Sample : K5710-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP- 32-S

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-BF110619.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

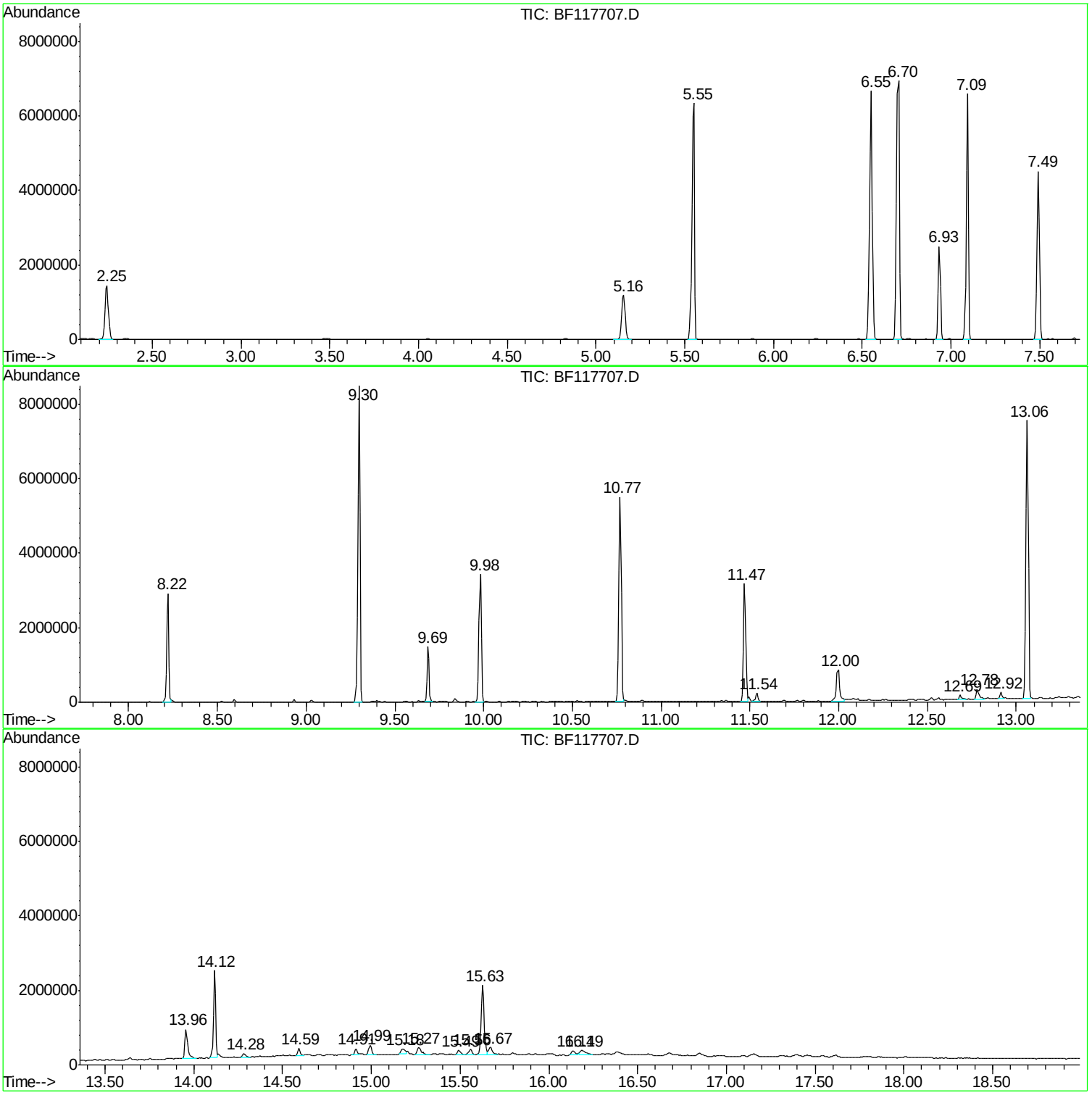
Sum of corrected areas: 74163520

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117707.D
Acq On : 7 Nov 2019 16:26
Operator : JU
Sample : K5710-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP- 32-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117707.D
Acq On : 7 Nov 2019 16:26
Operator : JU
Sample : K5710-07
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ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP- 32-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

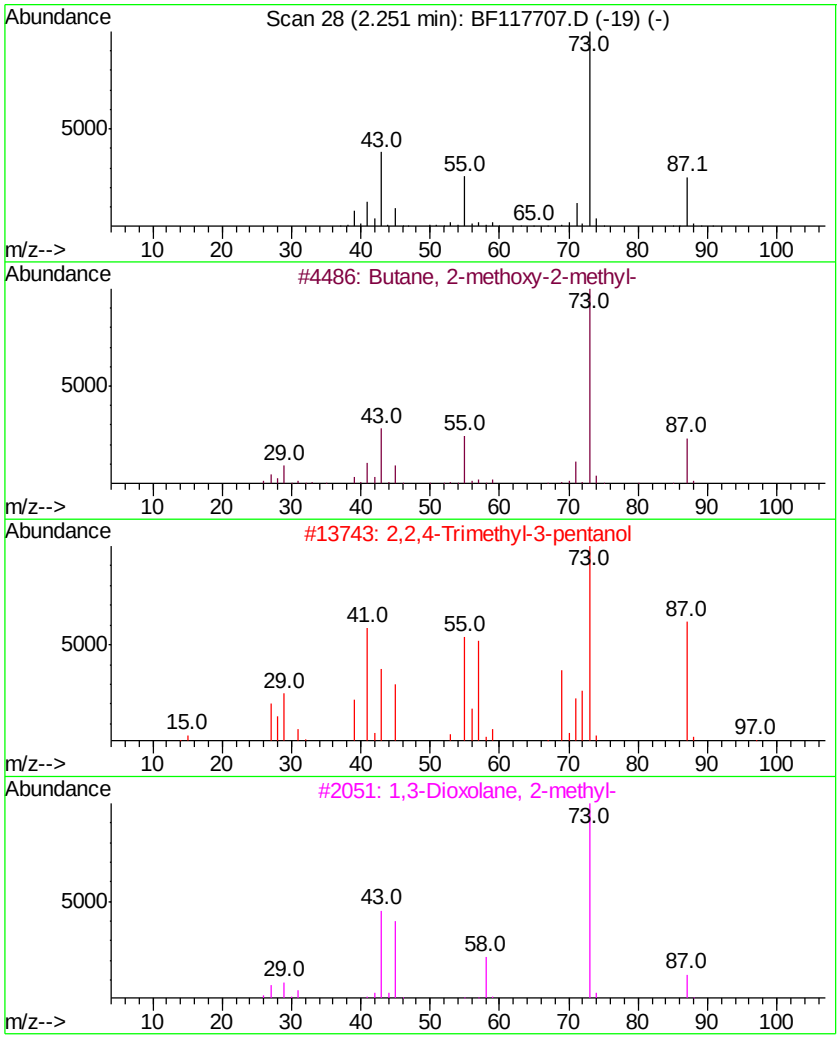
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

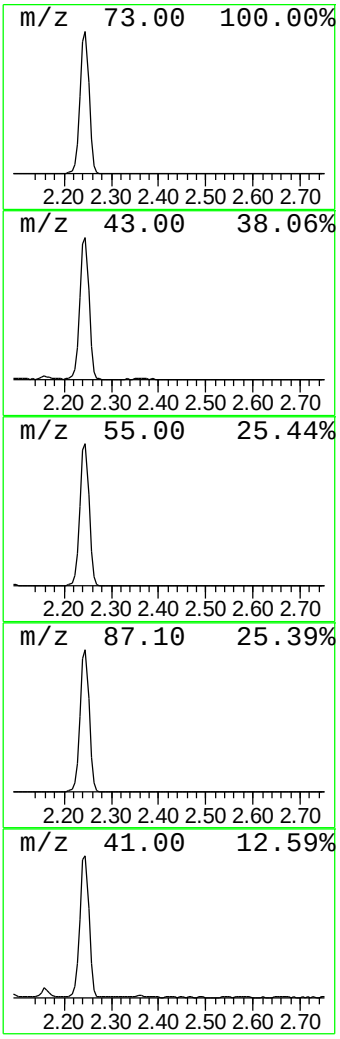
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	19.87 ng	1915940	1,4-Dichlorobenzene-d4	6.93

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	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117707.D
Acq On : 7 Nov 2019 16:26
Operator : JU
Sample : K5710-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP- 32-S

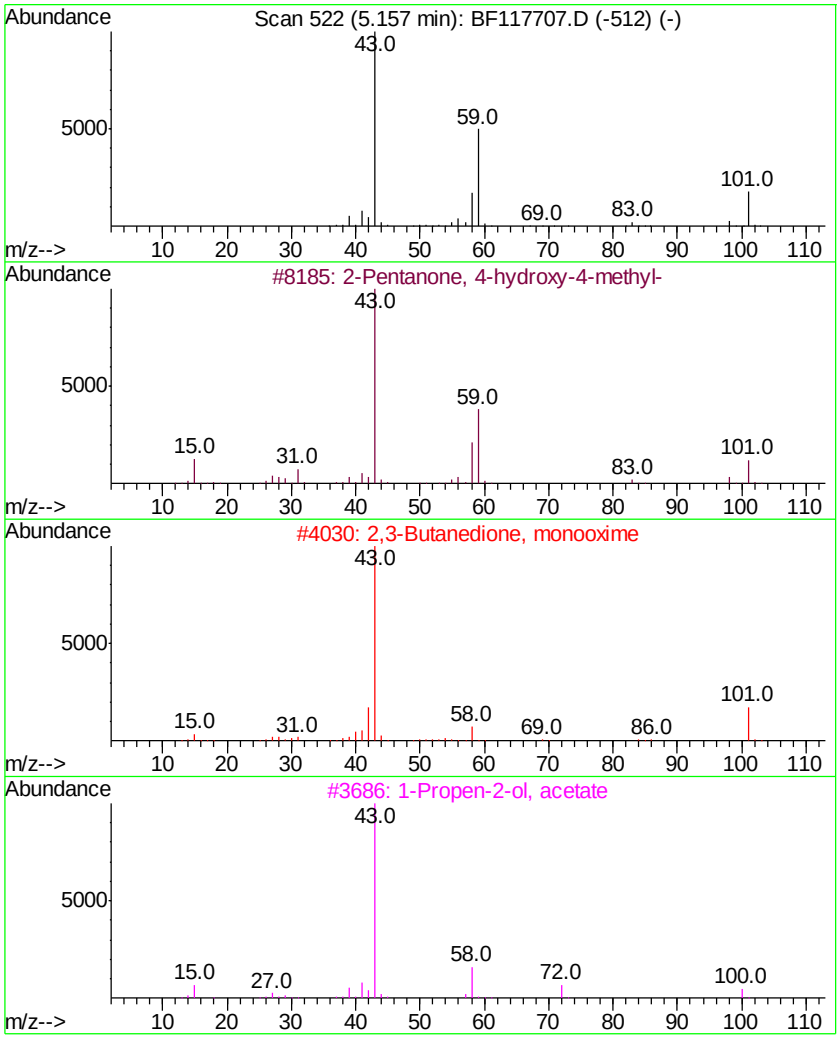
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

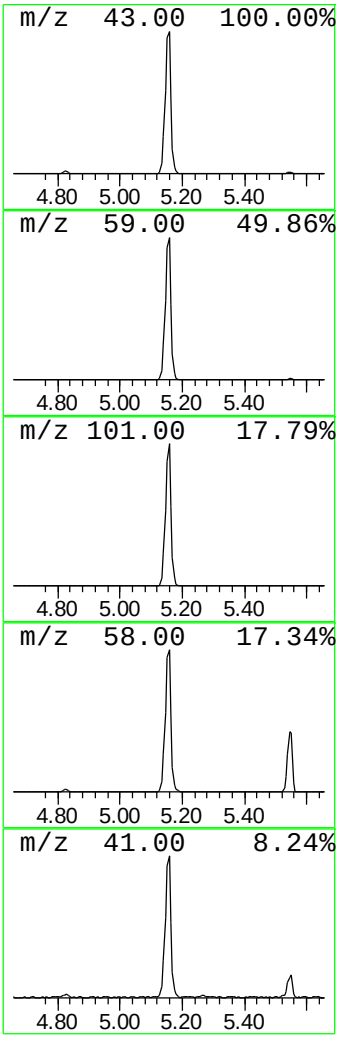
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	15.76 ng	1519620	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117707.D
Acq On : 7 Nov 2019 16:26
Operator : JU
Sample : K5710-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP- 32-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

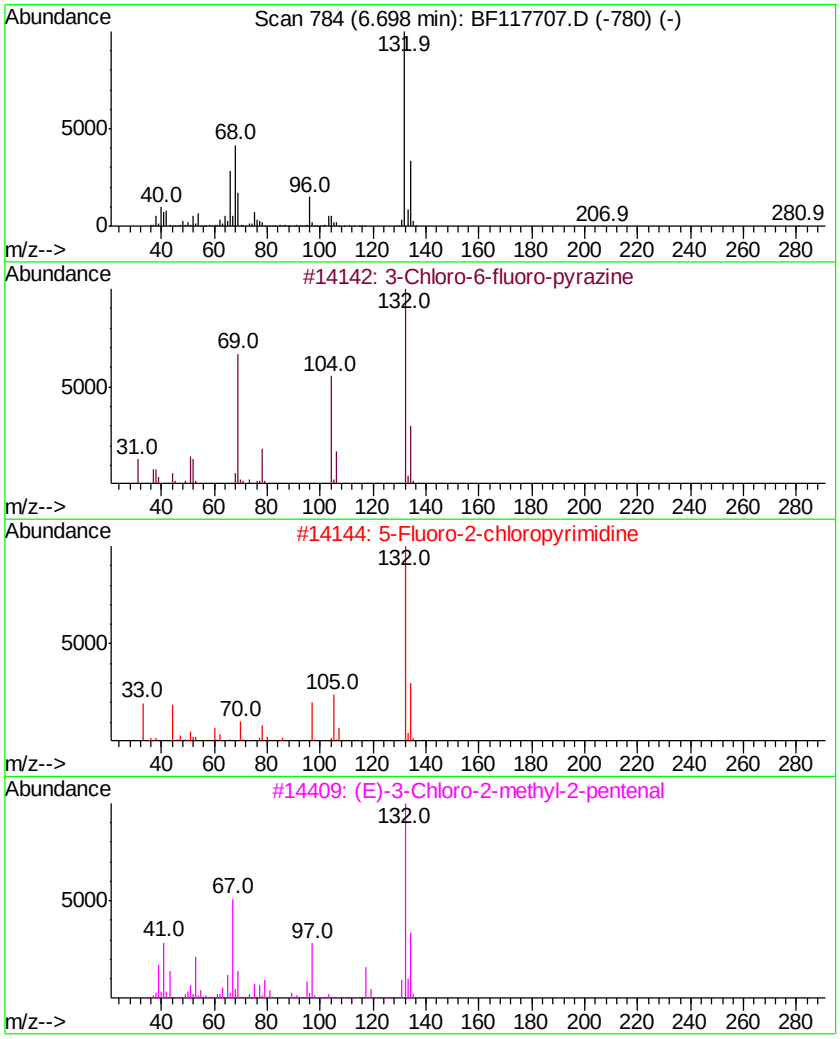
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

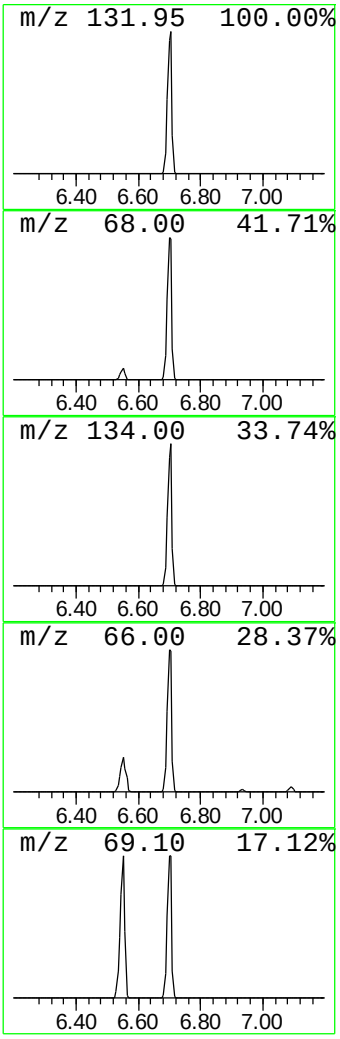
****

Peak Number 3 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	73.94 ng	7128420	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117707.D
Acq On : 7 Nov 2019 16:26
Operator : JU
Sample : K5710-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP- 32-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

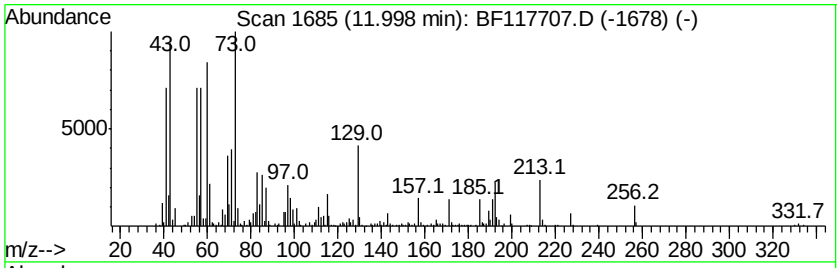
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

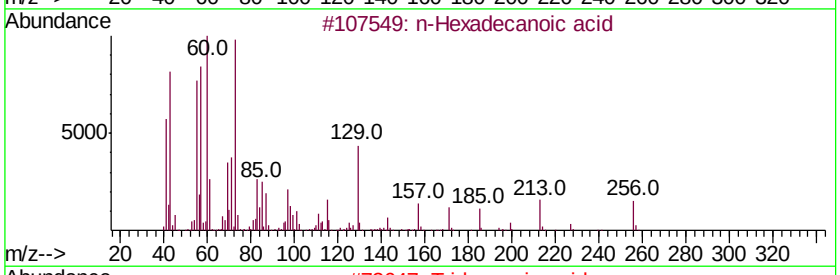
****

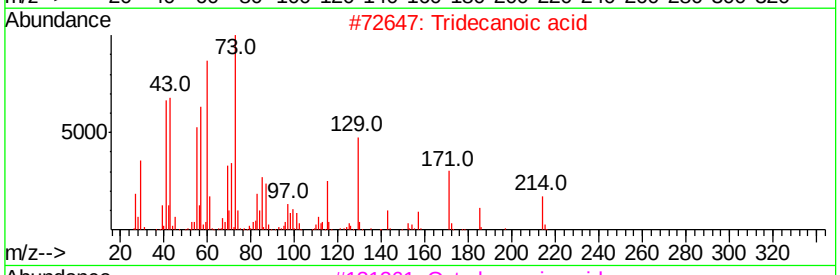
Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

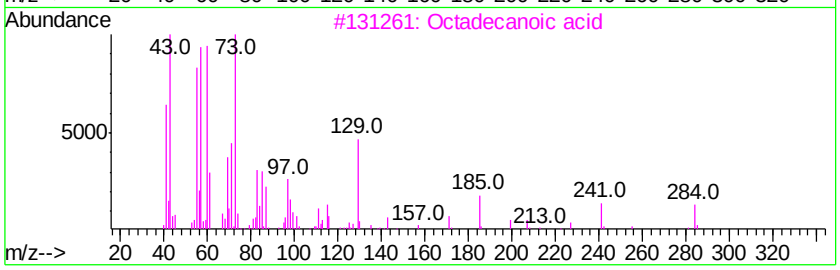
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	7.13 ng	988883	Phenanthrene-d10	11.47

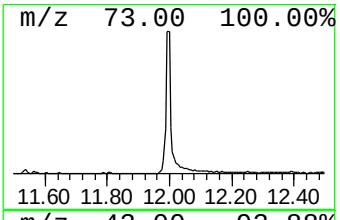
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Octadecanoic acid	284	C18H36O2	000057-11-4	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70

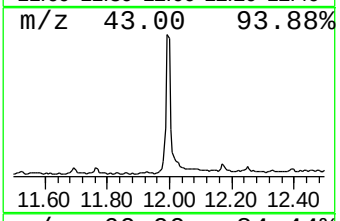


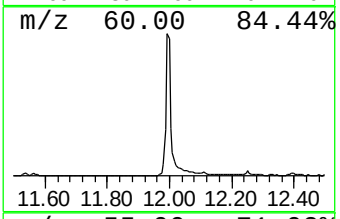


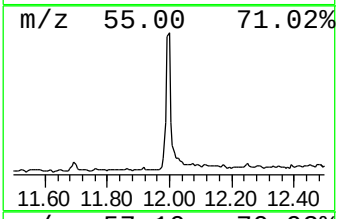


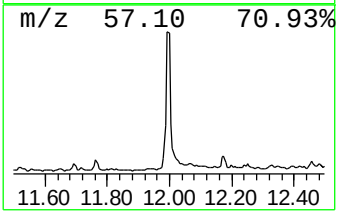












Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117707.D
Acq On : 7 Nov 2019 16:26
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Sample : K5710-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP- 32-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

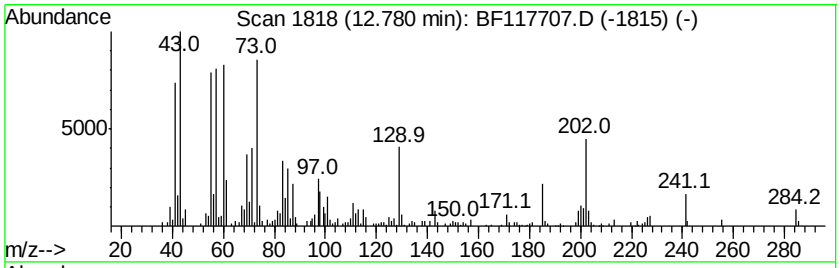
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

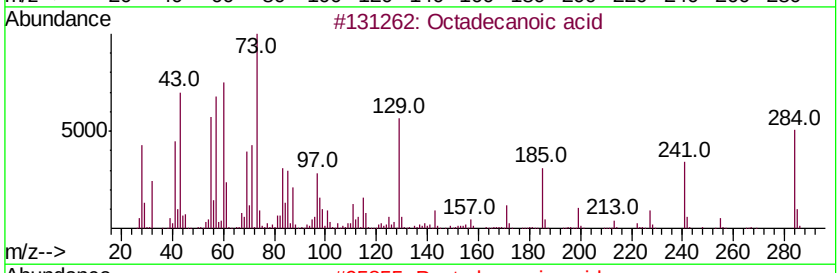
****

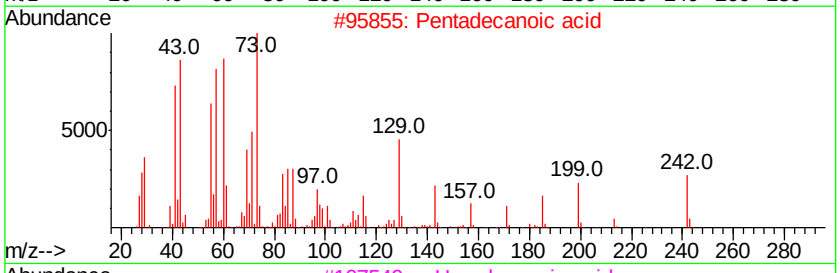
Peak Number 6 Octadecanoic acid Concentration Rank 9

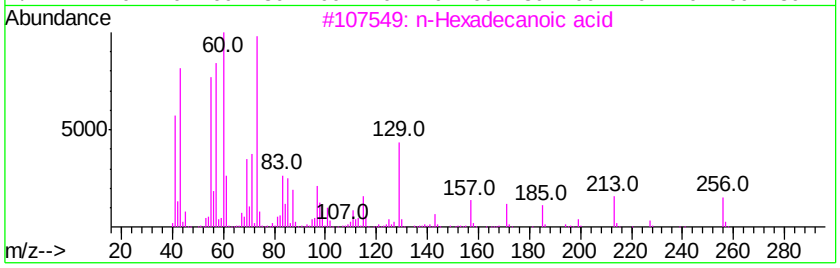
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	2.28 ng	316583	Phenanthrene-d10	11.47

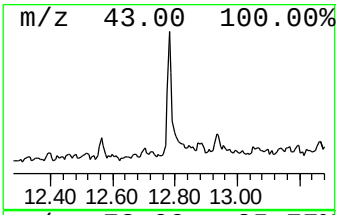
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
5	Dodecanoic acid	200	C12H24O2	000143-07-7	68

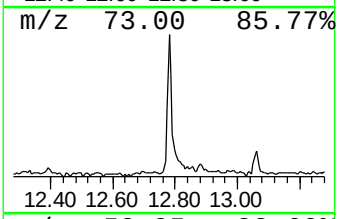


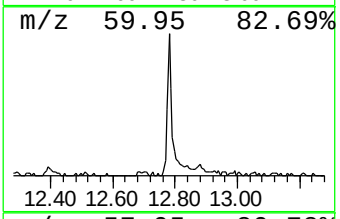


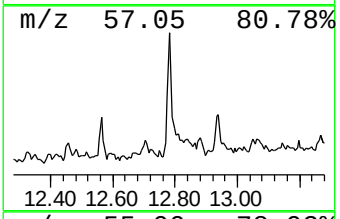


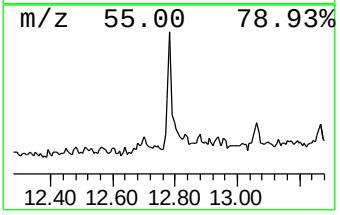












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP- 32-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

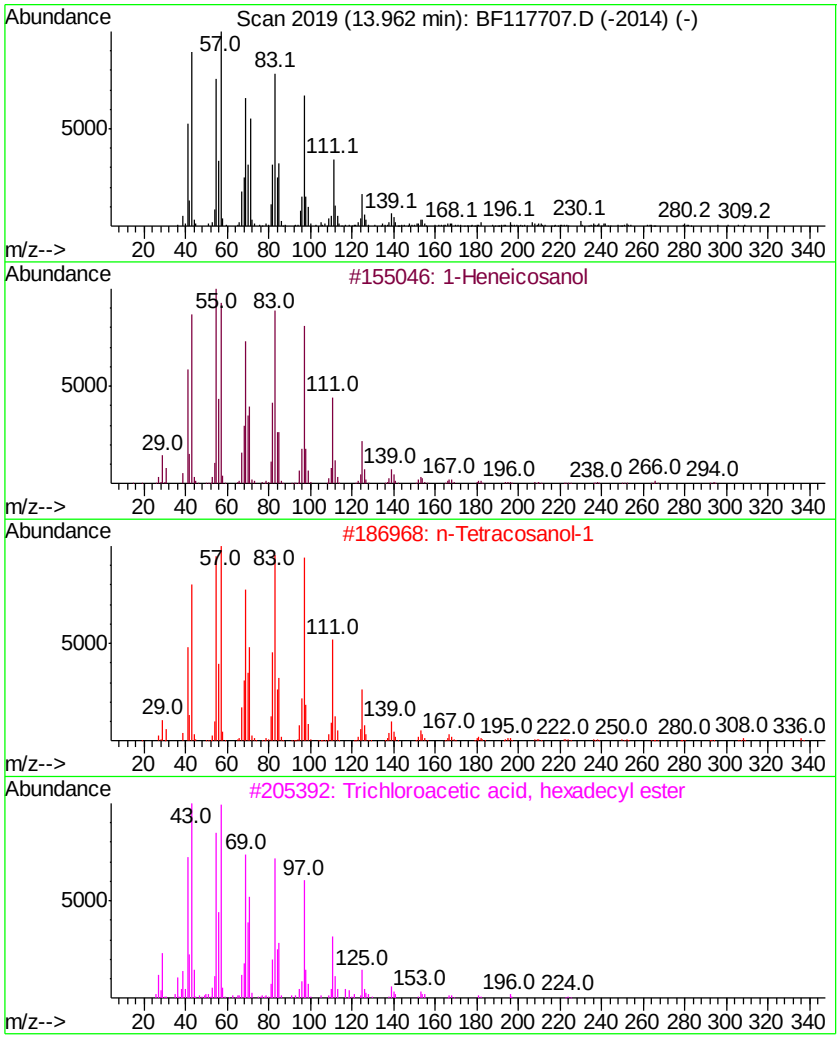
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

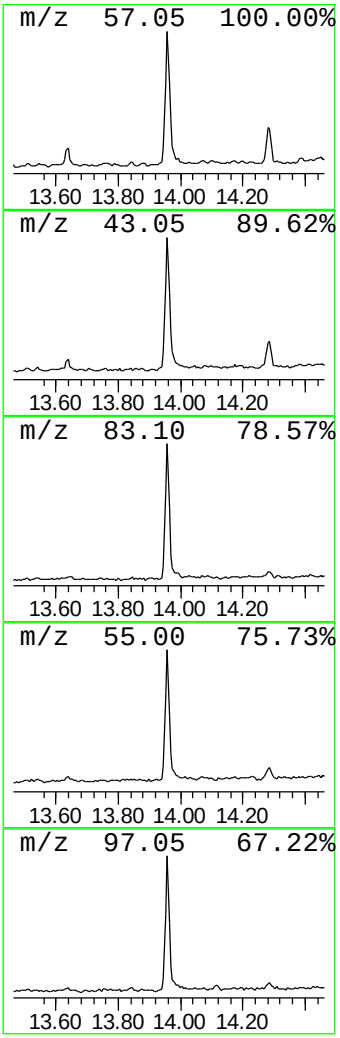
****

Peak Number 7 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	7.86 ng	825548	Chrysene-d12	14.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
5	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	93





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Operator : JU
Sample : K5710-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP- 32-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.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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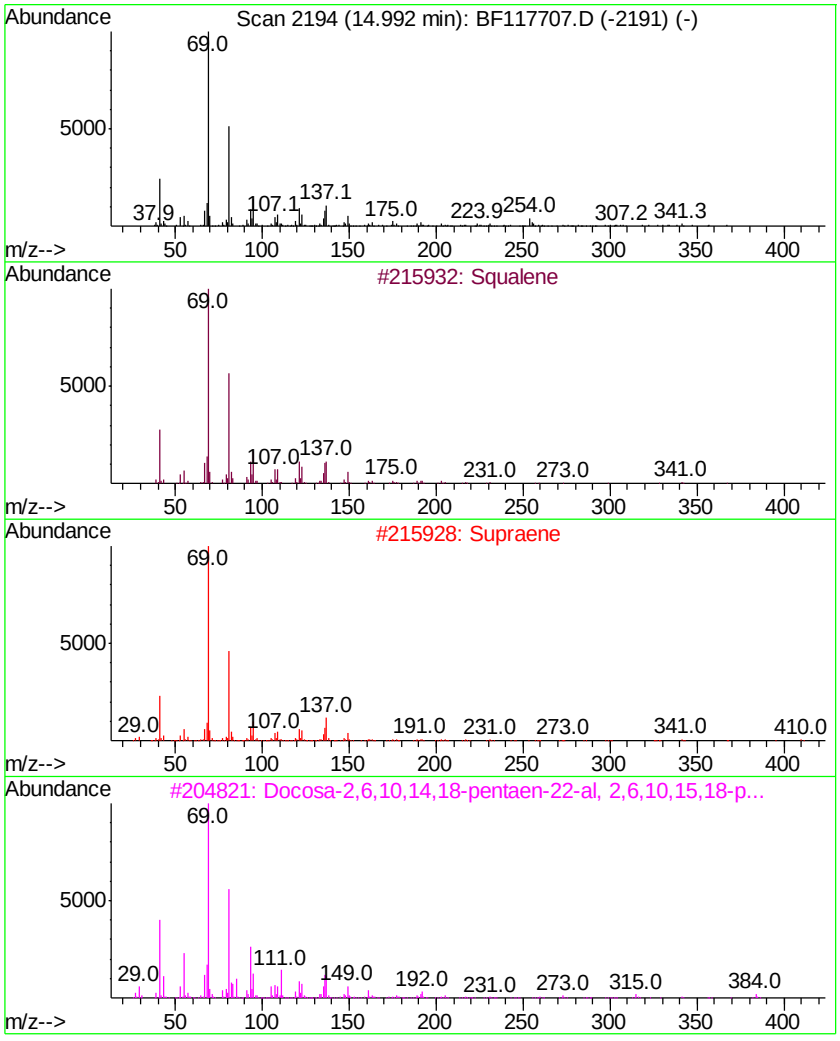
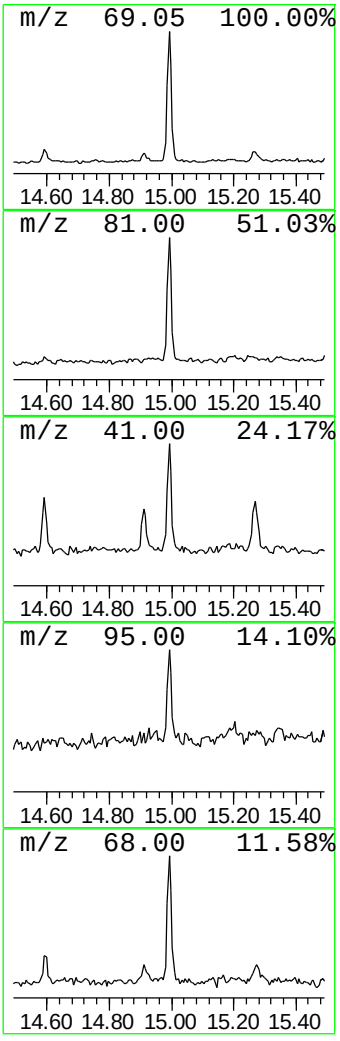
Peak Number 8 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	2.31 ng	265097	Perylene-d12	15.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	90
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	86
4	6,10,14-Hexadecatrien-1-ol, 3,7,...	292	C20H36O	036237-66-8	72
5	1-(Phenylthio)-3,7,11-trimethyl-...	314	C21H30S	028413-57-2	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117707.D
Acq On : 7 Nov 2019 16:26
Operator : JU
Sample : K5710-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP- 32-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.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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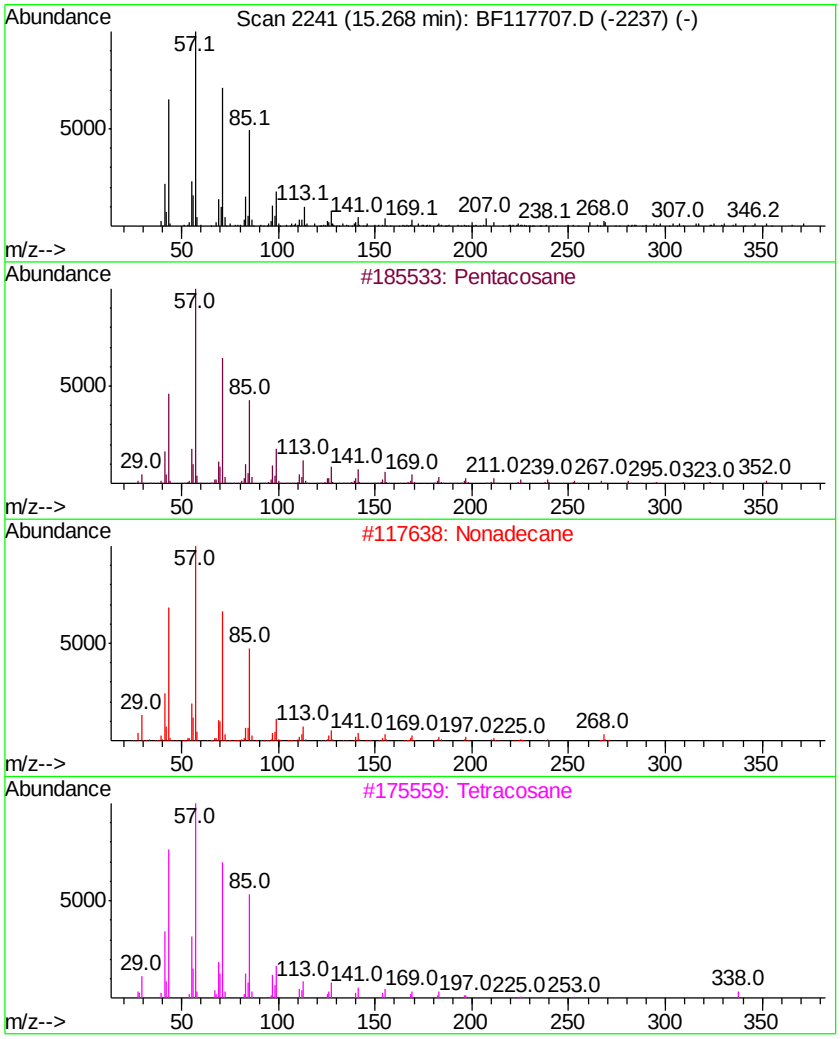
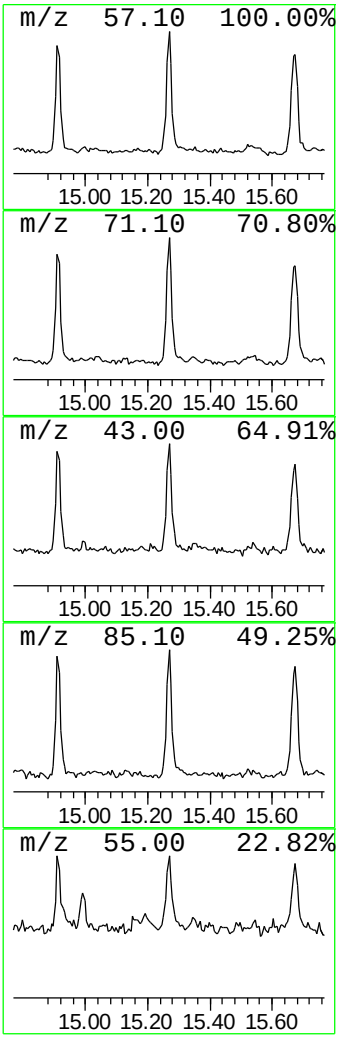
Peak Number 9 Pentacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	2.80 ng	320765	Perylene-d12	15.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	96
2	Nonadecane	268	C19H40	000629-92-5	96
3	Tetracosane	338	C24H50	000646-31-1	90
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
5	Heneicosane	296	C21H44	000629-94-7	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117707.D
Acq On : 7 Nov 2019 16:26
Operator : JU
Sample : K5710-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP- 32-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.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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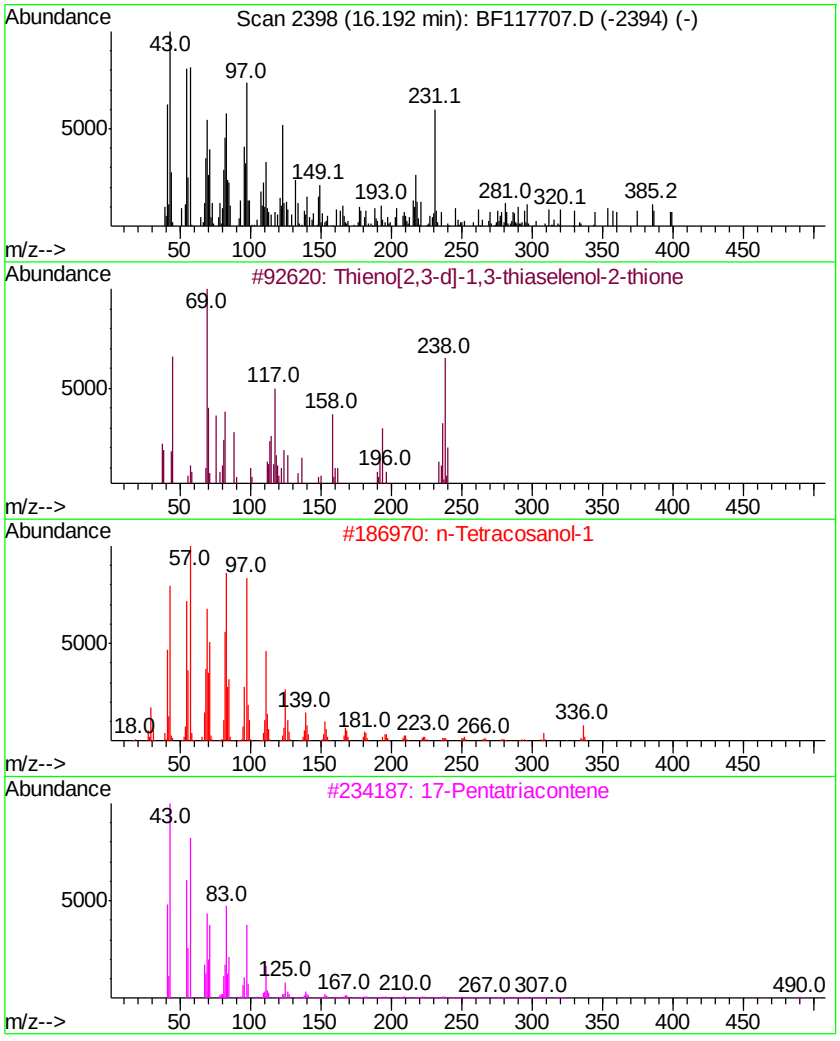
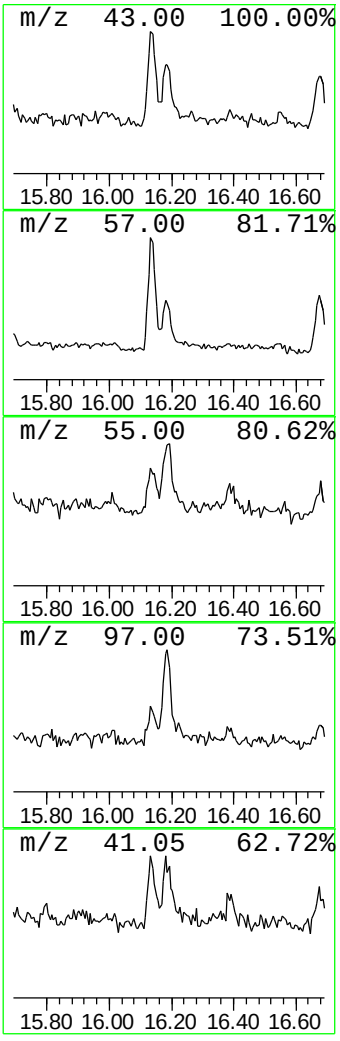
Peak Number 10 Thieno[2,3-d]-1,3-thiaselen... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	2.20 ng	252802	Perylene-d12	15.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thieno[2,3-d]-1,3-thiaselenol-2-...	238	C5H2S3Se	081803-09-0	56
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	55
3	17-Pentatriacontene	491	C35H70	006971-40-0	49
4	1-Heptacosanol	396	C27H56O	002004-39-9	49
5	1-Heneicosanol	312	C21H44O	015594-90-8	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110719\
Data File : BF117707.D
Acq On : 7 Nov 2019 16:26
Operator : JU
Sample : K5710-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP- 32-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.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...	2.25	19.9	ng	1915940	1	6.93	1928270	20.0
2-Pentanone, 4-hy...	5.16	15.8	ng	1519620	1	6.93	1928270	20.0
unknown6.70	6.70	73.9	ng	7128420	1	6.93	1928270	20.0
n-Hexadecanoic acid	12.00	7.1	ng	988883	4	11.47	2772780	20.0
Octadecanoic acid	12.78	2.3	ng	316583	4	11.47	2772780	20.0
1-Heneicosanol	13.96	7.9	ng	825548	5	14.12	2100570	20.0
Squalene	14.99	2.3	ng	265097	6	15.63	2293350	20.0
Pentacosane	15.27	2.8	ng	320765	6	15.63	2293350	20.0
Thieno[2,3-d]-1,3...	16.19	2.2	ng	252802	6	15.63	2293350	20.0