LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
Data File : BF117619.D
Acq On : 30 Oct 2019 12:53
Operator : JU
Sample : K5539-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 164-10-(0-1)

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-BF101819.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	4.928	480	483	498	rBV	29053	49245	4.85%	0.572%
2	5.357	552	556	577	rBV	688658	896375	88.24%	10.406%
3	6.386	727	731	747	rBV	841008	1012456	99.67%	11.754%
4	6.504	747	751	759	rVB	1107970	1015838	100.00%	11.793%
5	6.728	786	789	800	rBV	230939	215946	21.26%	2.507%
6	6.881	812	815	830	rBV	793686	702799	69.18%	8.159%
7	7.292	882	885	911	rBV	486076	598420	58.91%	6.947%
8	8.010	1003	1007	1022	rBV	226015	271152	26.69%	3.148%
9	9.080	1185	1189	1201	rBV	1051048	970598	95.55%	11.268%
10	9.480	1254	1257	1268	rBV	69173	77047	7.58%	0.894%
11	9.757	1301	1304	1320	rBB	294847	308941	30.41%	3.587%
12	10.557	1436	1440	1455	rBV	482970	540452	53.20%	6.274%
13	11.251	1554	1558	1567	rBV	239974	274599	27.03%	3.188%
14	11.774	1644	1647	1655	rBV2	32264	36092	3.55%	0.419%
15	12.468	1761	1765	1770	rBV	18936	19650	1.93%	0.228%
16	12.698	1798	1804	1809	rBV	18111	20628	2.03%	0.239%
17	12.827	1822	1826	1832	rBV	838864	739796	72.83%	8.588%
18	13.733	1976	1980	1988	rBV7	29742	52788	5.20%	0.613%
19	13.892	2003	2007	2018	rBV	225058	253487	24.95%	2.943%
20	14.345	2081	2084	2086	rVB2	23675	19334	1.90%	0.224%
21	14.639	2132	2134	2140	rVB2	32096	37424	3.68%	0.434%
22	14.709	2143	2146	2150	rBV	66003	62465	6.15%	0.725%
23	14.927	2181	2183	2185	rBV3	11491	12736	1.25%	0.148%
24	14.957	2185	2188	2192	rVB	52195	54755	5.39%	0.636%
25	15.333	2244	2252	2258	rVB	174210	269689	26.55%	3.131%
26	15.715	2313	2317	2320	rVB	32684	40954	4.03%	0.475%
27	15.939	2353	2355	2364	rVB9	13339	29835	2.94%	0.346%
28	16.180	2394	2396	2401	rVB5	20478	30359	2.99%	0.352%

Sum of corrected areas: 8613860

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
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Operator : JU
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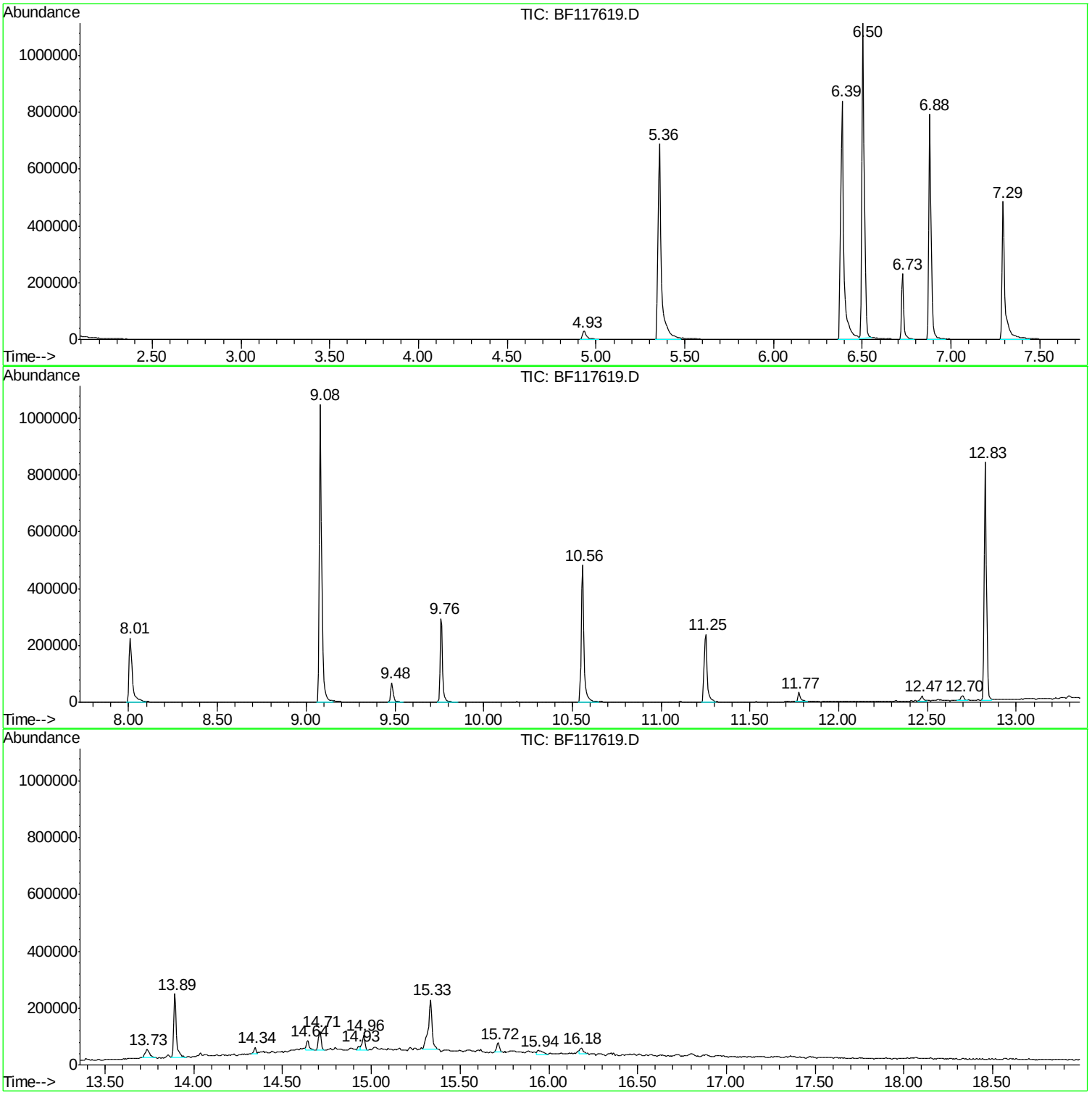
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
164-10-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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\BF103019\
Data File : BF117619.D
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Operator : JU
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Instrument : BNA_F
ClientSampleId : 164-10-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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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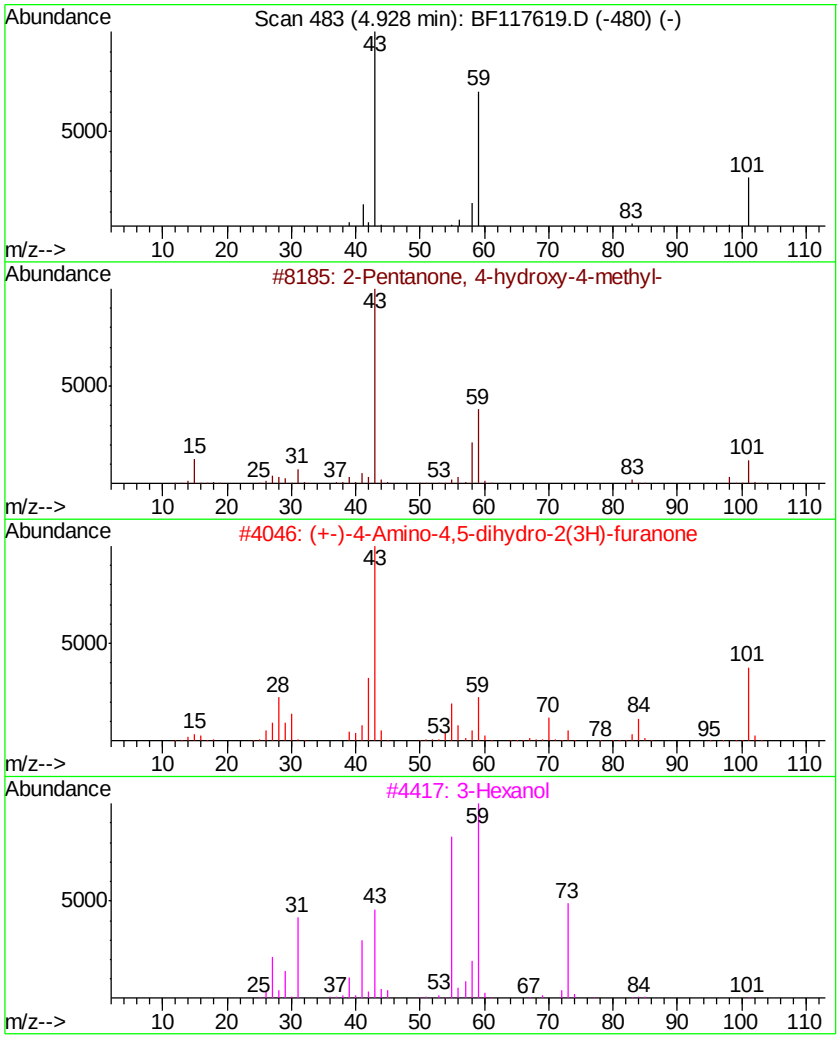
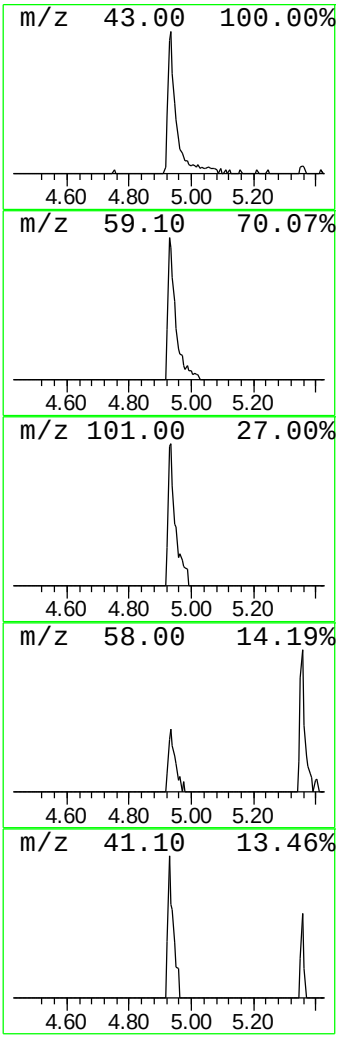
Peak Number 1 unknown4.93 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	4.56 ng	49245	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	28
3	3-Hexanol	102	C6H14O	000623-37-0	25
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

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Data File : BF117619.D
Acq On : 30 Oct 2019 12:53
Operator : JU
Sample : K5539-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 164-10-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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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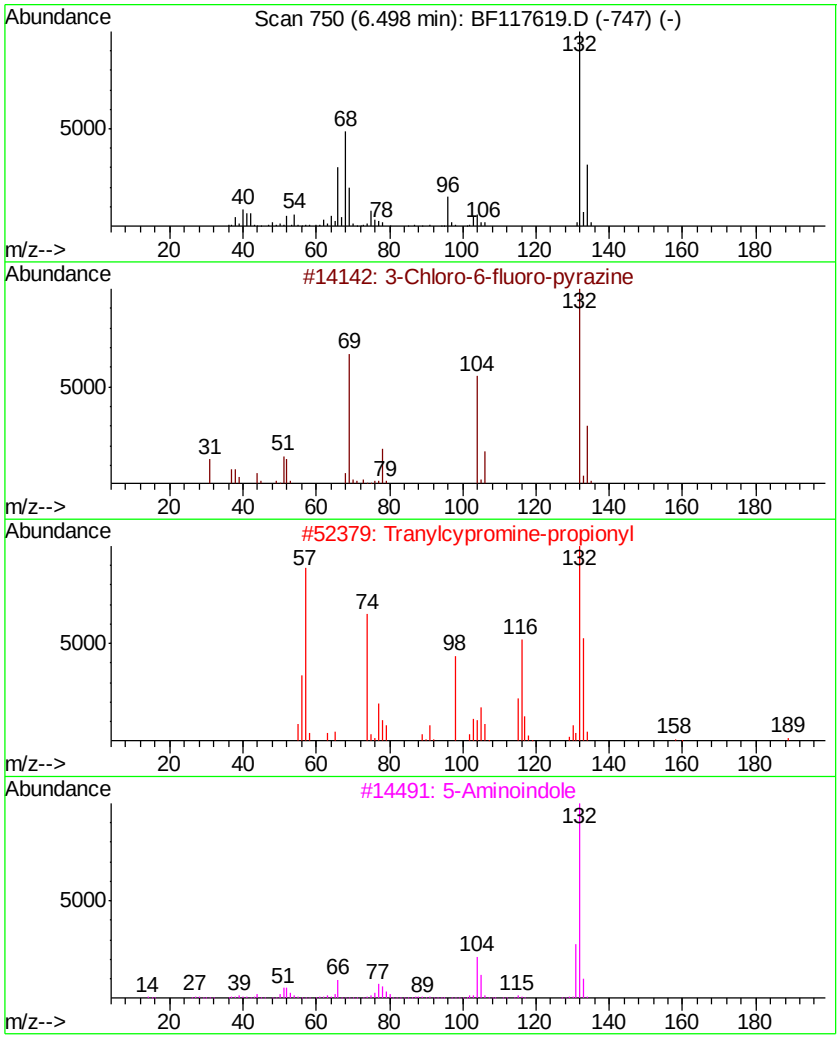
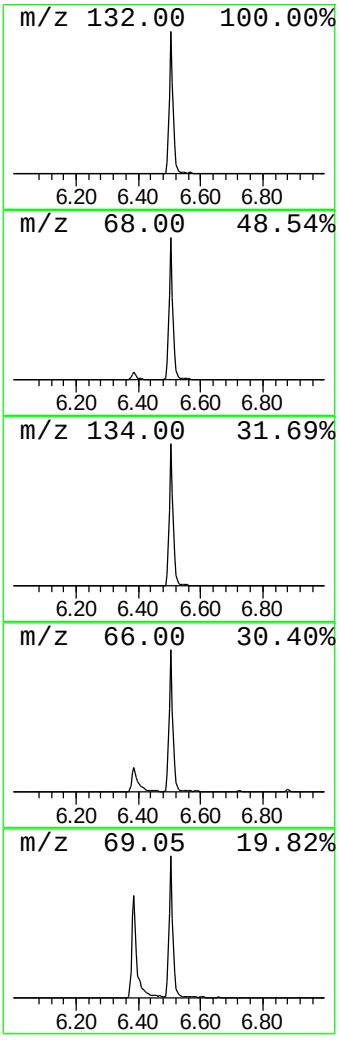
Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	94.08 ng	1015840	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
Data File : BF117619.D
Acq On : 30 Oct 2019 12:53
Operator : JU
Sample : K5539-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 164-10-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
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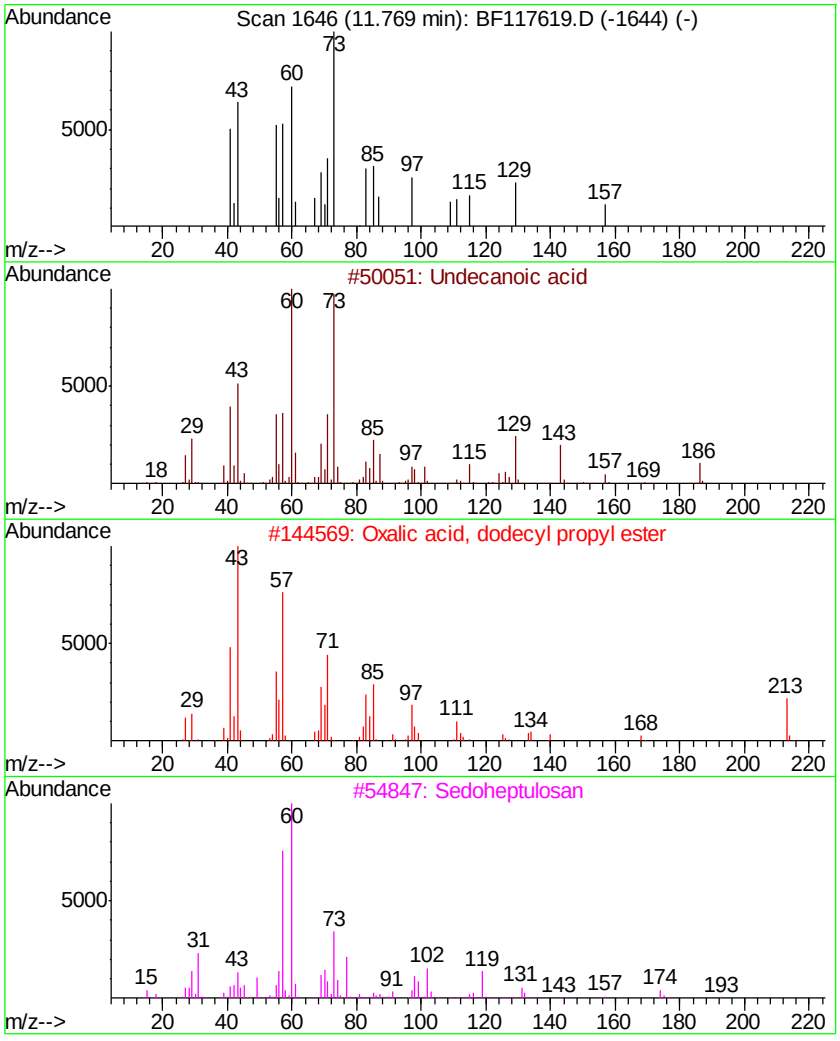
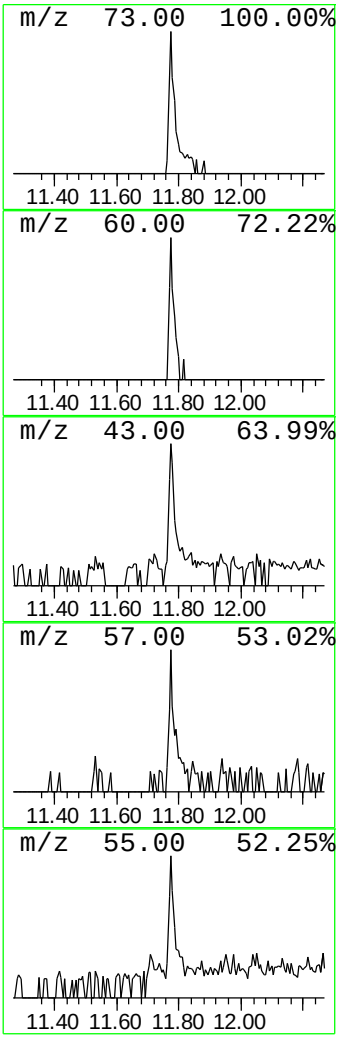
Peak Number 4 unknown11.77 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	2.63 ng	36092	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	47
2	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	22
3	Sedoheptulosan	192	C7H12O6	000469-90-9	22
4	2-Piperidinone, N-[4-bromo-n-but...	233	C9H16BrNO	195194-80-0	14
5	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	14





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Operator : JU
Sample : K5539-13
Misc :
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Instrument : BNA_F
ClientSampleId : 164-10-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

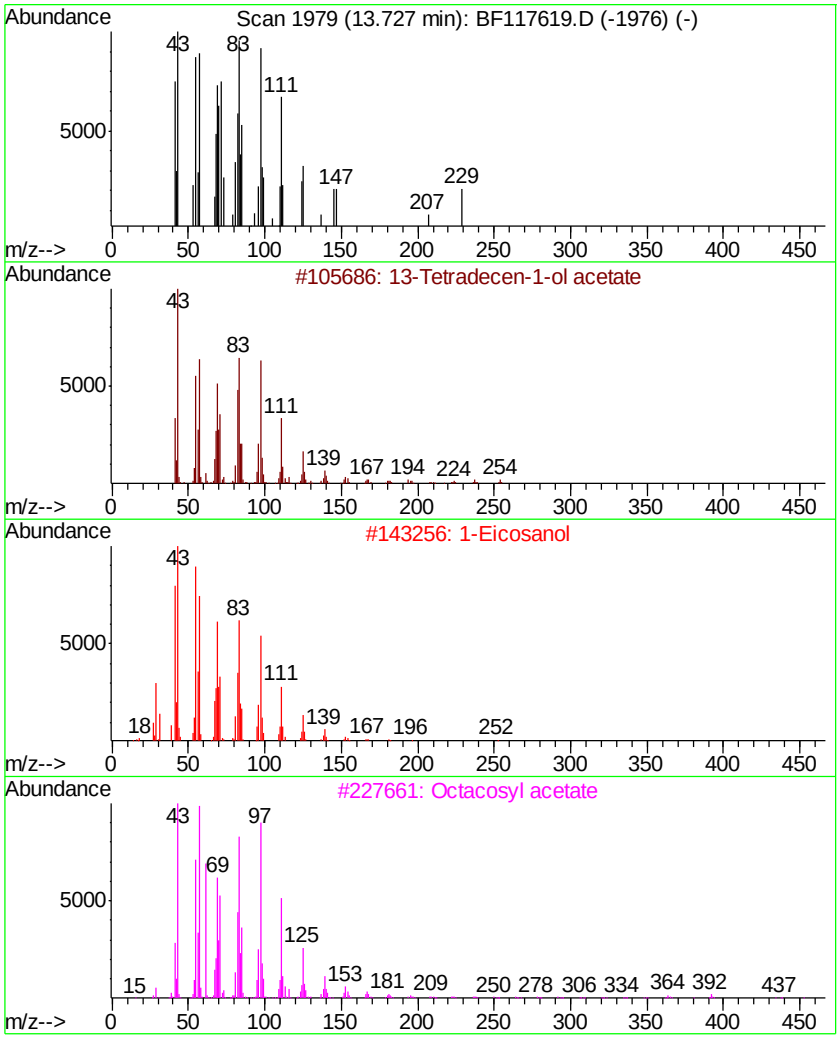
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

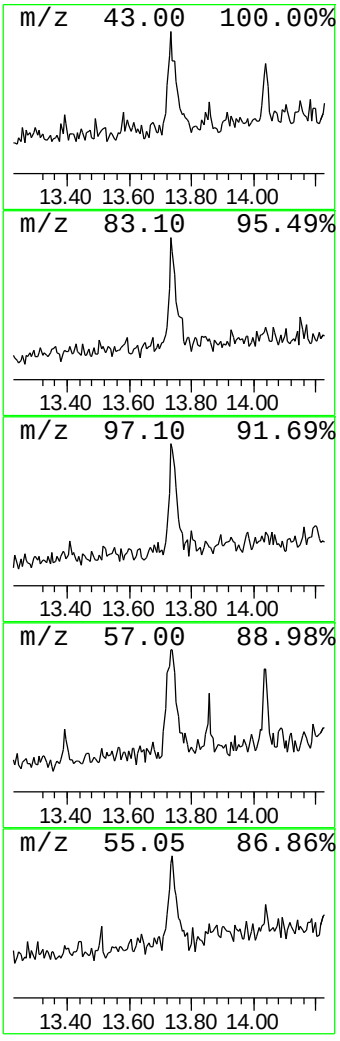
****

Peak Number 5 13-Tetradecen-1-ol acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	4.16 ng	52788	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	90
2	1-Eicosanol	298	C20H42O	000629-96-9	87
3	Octacosyl acetate	452	C30H60O2	018206-97-8	86
4	11-Tricosene	322	C23H46	052078-56-5	83
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	80





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 164-10-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
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TIC Library : C:\DATABASE\NIST11.L
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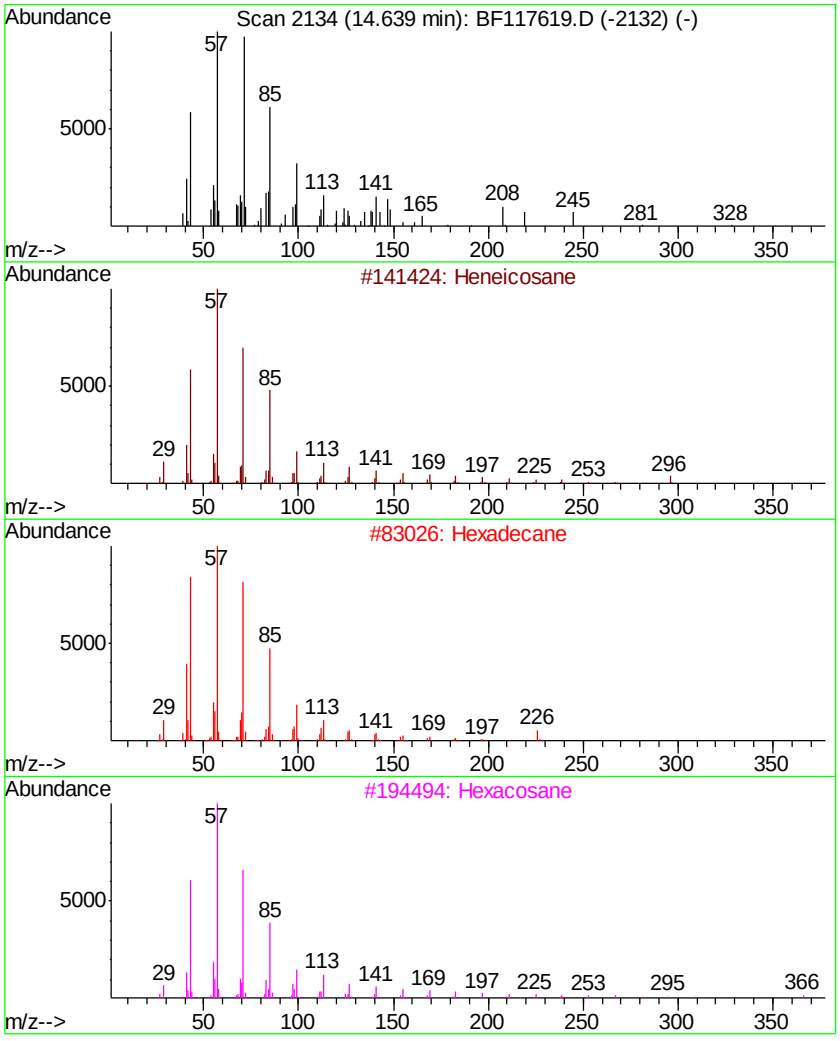
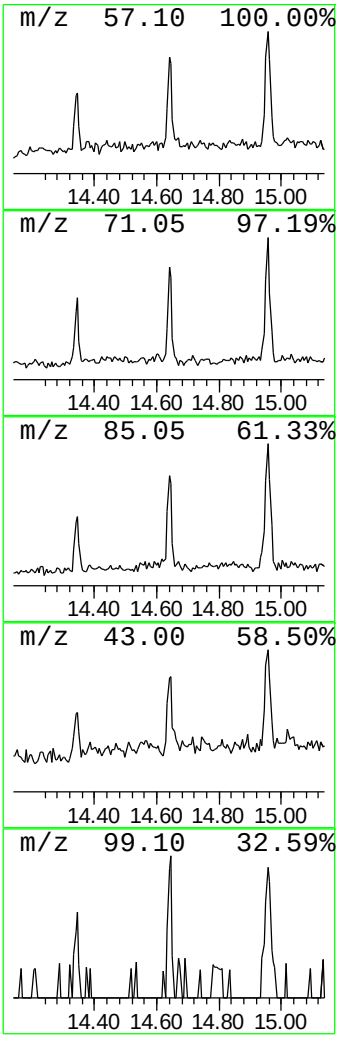
Peak Number 6 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.78 ng	37424	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	64
2	Hexadecane	226	C16H34	000544-76-3	59
3	Hexacosane	366	C26H54	000630-01-3	59
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	50
5	Nonane, 5-butyl-	184	C13H28	017312-63-9	47





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 164-10-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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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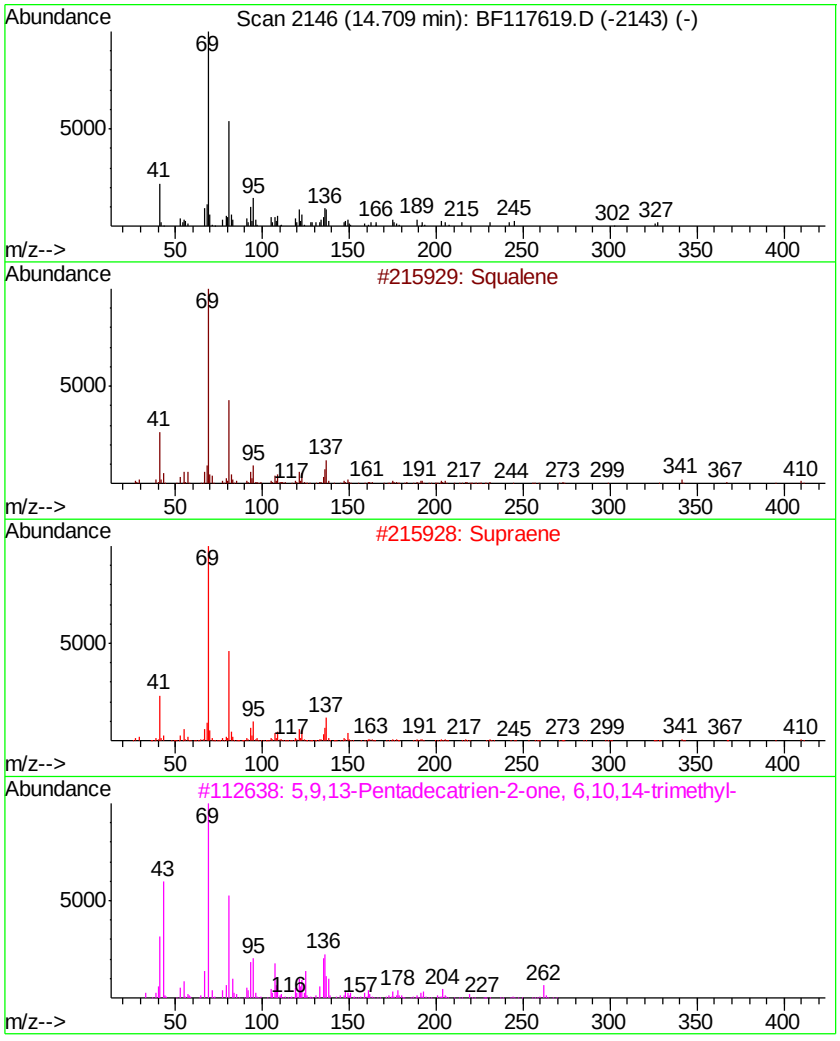
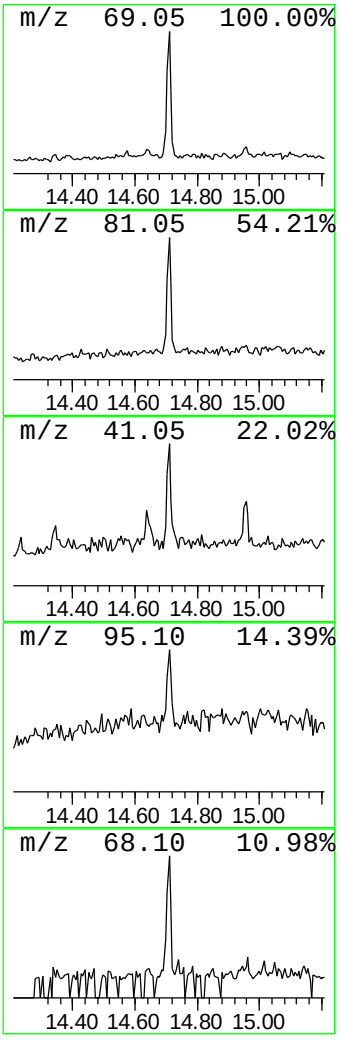
Peak Number 7 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	4.63 ng	62465	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	80
2	Supraene	410	C30H50	007683-64-9	72
3	5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	000762-29-8	64
4	2-Propenoic acid, 2-methyl-, 2-p...	124	C7H8O2	013861-22-8	53
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	53





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : 164-10-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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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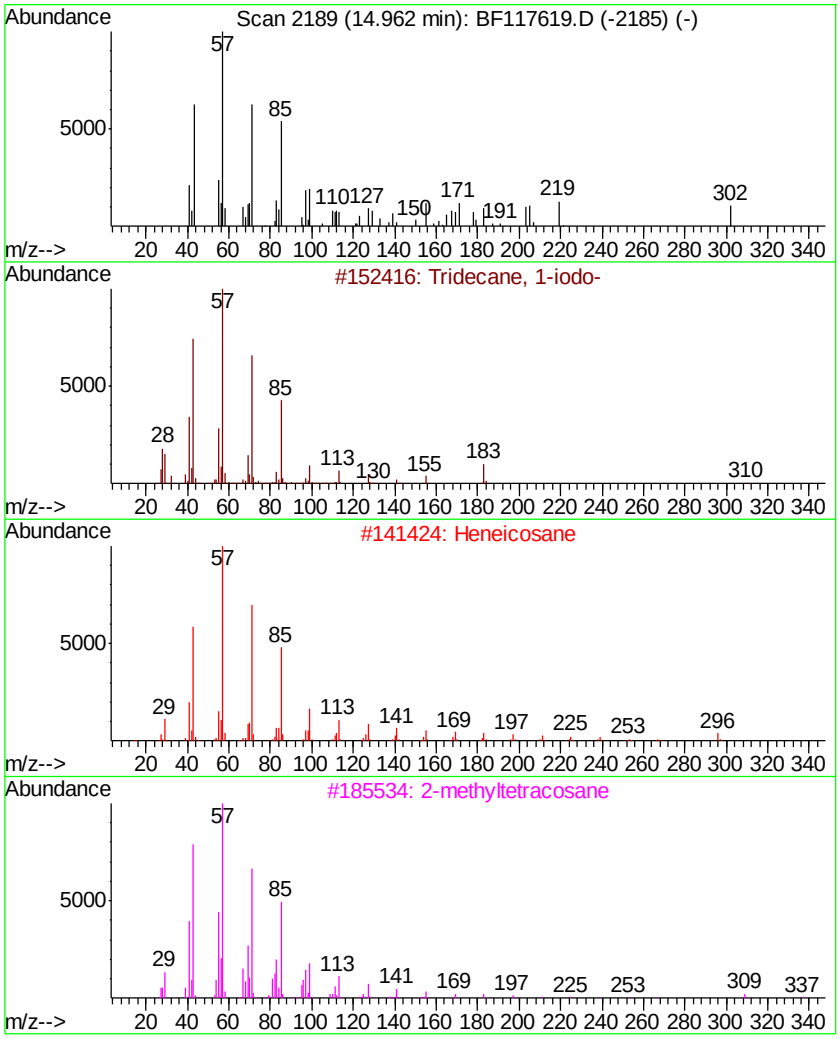
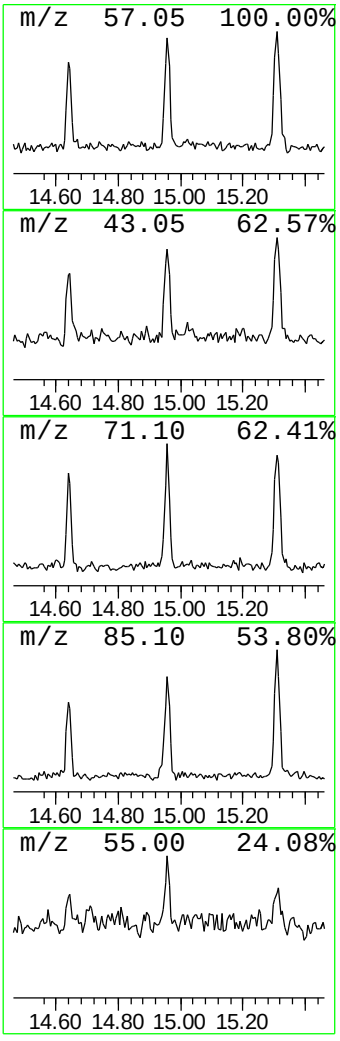
Peak Number 8 Tridecane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	4.06 ng	54755	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	72
2	Heneicosane	296	C21H44	000629-94-7	72
3	2-methyltetracosane	352	C25H52	1000376-72-6	72
4	Eicosane	282	C20H42	000112-95-8	72
5	Tetratetracontane	619	C44H90	007098-22-8	72





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Instrument : BNA_F
ClientSampleId : 164-10-(0-1)

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TIC Library : C:\DATABASE\NIST11.L
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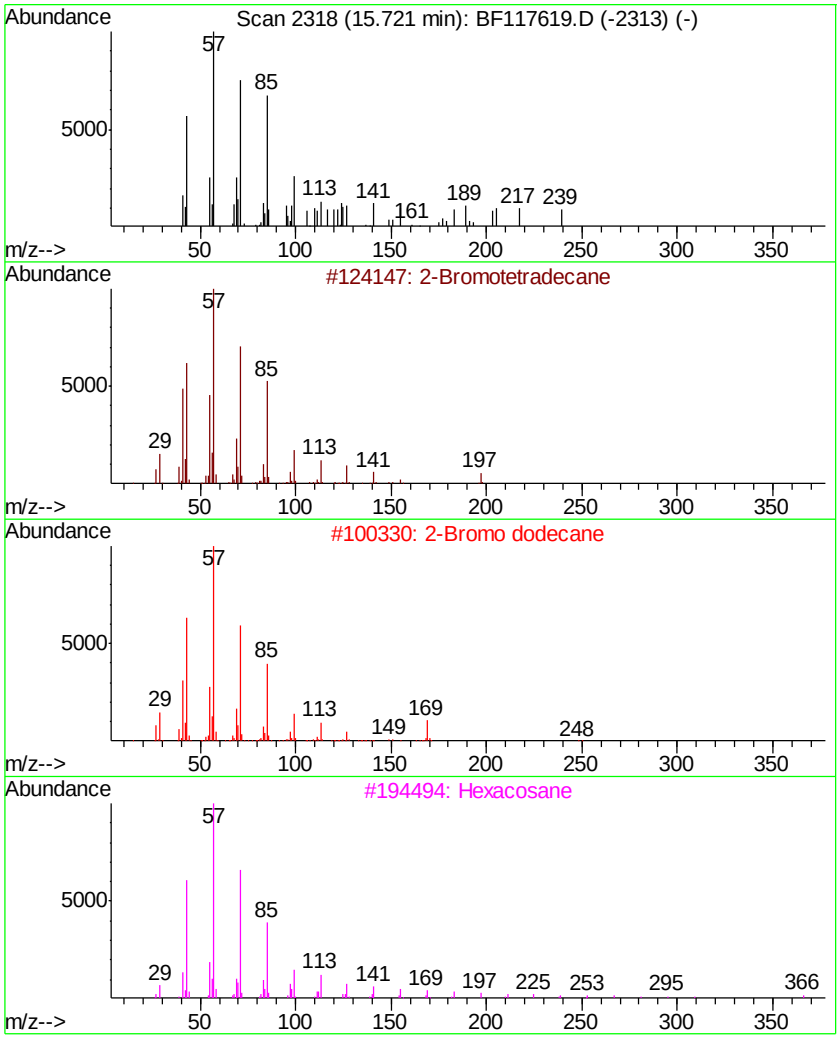
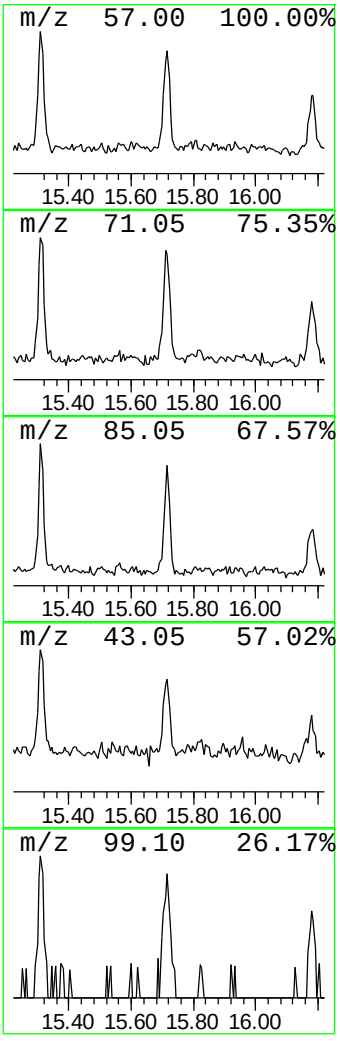
Peak Number 9 2-Bromotetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	3.04 ng	40954	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromotetradecane	276	C14H29Br	074036-95-6	86
2	2-Bromo dodecane	248	C12H25Br	013187-99-0	78
3	Hexacosane	366	C26H54	000630-01-3	53
4	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	53
5	Heneicosane	296	C21H44	000629-94-7	50





Library Search Compound Report

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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 164-10-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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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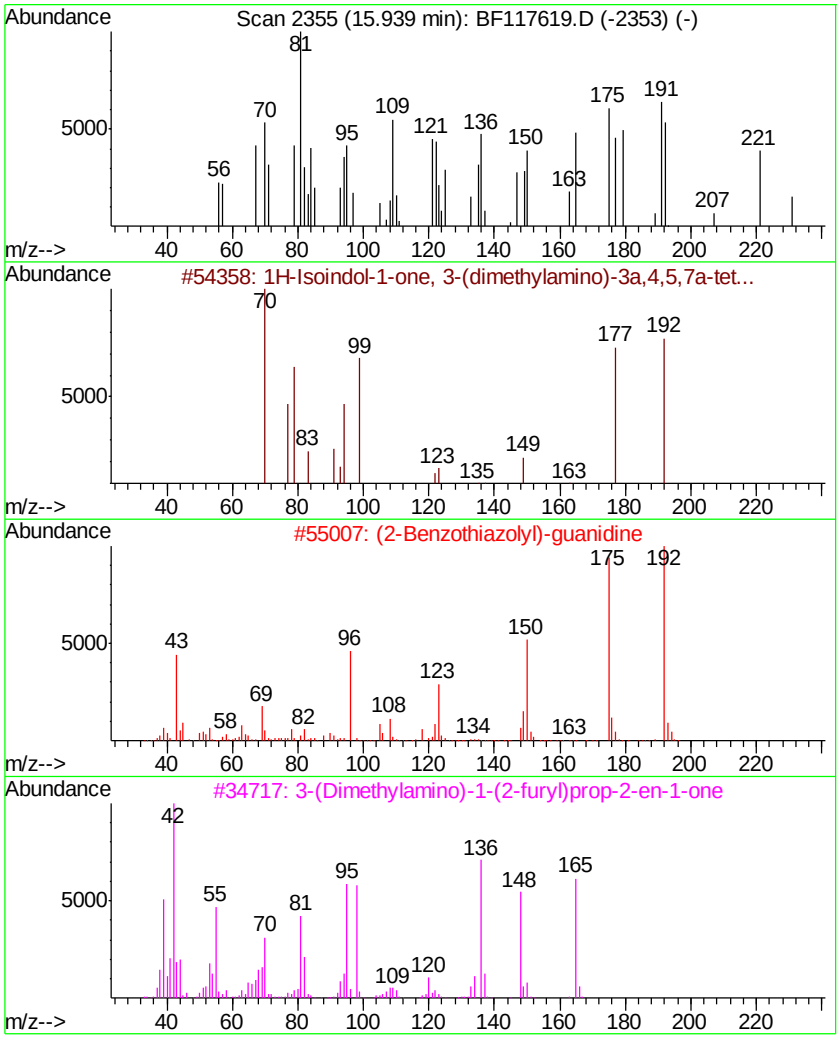
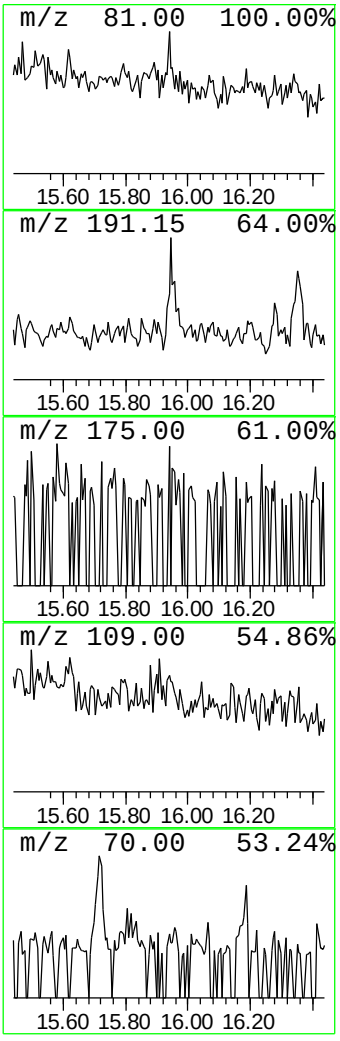
Peak Number 10 unknown15.94 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	2.21 ng	29835	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Isoindol-1-one, 3-(dimethylam...	192	C11H16N2O	075378-97-1	25
2	(2-Benzothiazolyl)-guanidine	192	C8H8N4S	002582-07-2	14
3	3-(Dimethylamino)-1-(2-furyl)pro...	165	C9H11NO2	017168-45-5	10
4	9-Borabicyclo[3.3.1]nonane, 9-(1...	192	C13H25B	121194-78-3	10
5	1,3-Butanedione, 1-(4-methoxyphe...	192	C11H12O3	004023-80-7	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
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Instrument : BNA_F
ClientSampleId : 164-10-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
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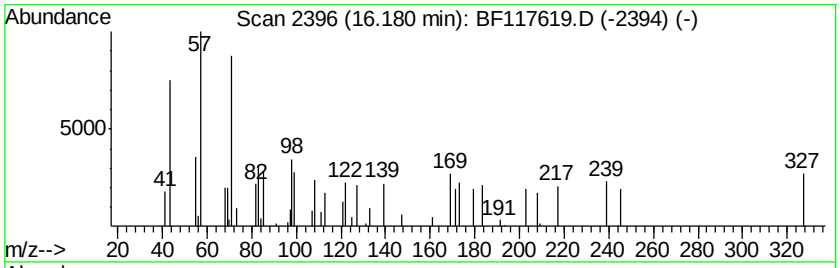
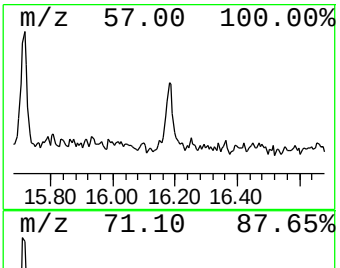
Peak Number 11 unknown16.18 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	2.25 ng	30359	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,5-Dibutylnonane	240	C17H36	006008-17-9	16
2	Hexadecane, 2,6,10-trimethyl-	268	C19H40	055000-52-7	16
3	Octadecane, 3-methyl-	268	C19H40	006561-44-0	16
4	Dodecane, 2-methyl-8-propyl-	226	C16H34	055045-07-3	16
5	Sulfurous acid, heptadecyl 2-pen...	390	C22H46O3S	1000309-16-7	16





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF103019\
Data File : BF117619.D
Acq On : 30 Oct 2019 12:53
Operator : JU
Sample : K5539-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 164-10-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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
unknown4.93	4.93	4.6	ng	49245	1	6.73	215946	20.0
unknown6.50	6.50	94.1	ng	1015840	1	6.73	215946	20.0
unknown11.77	11.77	2.6	ng	36092	4	11.25	274599	20.0
13-Tetradecen-1-o...	13.73	4.2	ng	52788	5	13.89	253487	20.0
Heneicosane	14.64	2.8	ng	37424	6	15.33	269689	20.0
Squalene	14.71	4.6	ng	62465	6	15.33	269689	20.0
Tridecane, 1-iodo-	14.96	4.1	ng	54755	6	15.33	269689	20.0
2-Bromotetradecane	15.72	3.0	ng	40954	6	15.33	269689	20.0
unknown15.94	15.94	2.2	ng	29835	6	15.33	269689	20.0
unknown16.18	16.18	2.3	ng	30359	6	15.33	269689	20.0