LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101019\
Data File : BF117363.D
Acq On : 10 Oct 2019 16:42
Operator : JU
Sample : K5297-14
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

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-BF091319.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	5.004	492	496	512	rBV	36325	51536	5.32%	0.523%
2	5.422	563	567	587	rBV	639524	800154	82.60%	8.125%
3	6.440	736	740	753	rBV	799130	894202	92.31%	9.080%
4	6.569	758	762	773	rVV	1031378	914641	94.42%	9.287%
5	6.792	797	800	810	rBV	269057	251855	26.00%	2.557%
6	6.951	823	827	842	rBV	694263	651947	67.30%	6.620%
7	7.357	892	896	922	rBV	430395	527159	54.42%	5.353%
8	8.075	1015	1018	1050	rBV	245659	329149	33.98%	3.342%
9	9.151	1197	1201	1217	rBV	980187	968732	100.00%	9.837%
10	9.545	1265	1268	1278	rBV	127756	125859	12.99%	1.278%
11	9.828	1313	1316	1332	rBV	410911	398097	41.09%	4.042%
12	10.622	1447	1451	1467	rBV	563474	590425	60.95%	5.995%
13	11.316	1566	1569	1578	rBV	380601	403911	41.69%	4.101%
14	11.839	1655	1658	1667	rBV	67502	76484	7.90%	0.777%
15	11.951	1675	1677	1683	rVB2	25961	26680	2.75%	0.271%
16	12.051	1691	1694	1698	rBV2	47630	44985	4.64%	0.457%
17	12.169	1710	1714	1716	rVB2	14437	13021	1.34%	0.132%
18	12.251	1725	1728	1732	rBV2	15225	13117	1.35%	0.133%
19	12.333	1737	1742	1745	rBV4	13737	14518	1.50%	0.147%
20	12.533	1773	1776	1780	rBV	37473	37985	3.92%	0.386%
21	12.627	1788	1792	1796	rBV3	13252	17750	1.83%	0.180%
22	12.763	1810	1815	1822	rVB	39366	42365	4.37%	0.430%
23	12.898	1834	1838	1841	rBV	1094236	948374	97.90%	9.630%
24	13.469	1929	1935	1937	rVB6	11480	14574	1.50%	0.148%
25	13.792	1986	1990	2000	rBV2	127905	215583	22.25%	2.189%
26	13.963	2015	2019	2029	rBV	321589	347742	35.90%	3.531%
27	14.110	2040	2044	2047	rBV2	24247	33335	3.44%	0.338%
28	14.416	2093	2096	2099	rBV	43598	41437	4.28%	0.421%
29	14.716	2141	2147	2151	rBV2	68709	116460	12.02%	1.183%
30	15.045	2199	2203	2208	rVB	94757	108433	11.19%	1.101%
31	15.357	2253	2256	2261	rBV7	12560	26559	2.74%	0.270%
32	15.421	2261	2267	2281	rVB2	249252	430081	44.40%	4.367%
33	15.833	2332	2337	2342	rVB2	56598	84260	8.70%	0.856%
34	15.898	2345	2348	2354	rVV7	21427	36161	3.73%	0.367%

LSC Area Percent Report

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Instrument :
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ClientSampleId :
TP-6

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-BF091319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.074	2374	2378	2385	rVB5	32773	62841	6.49%	0.638%
36	16.315	2415	2419	2431	rVB6	35554	96233	9.93%	0.977%
37	16.492	2445	2449	2456	rVB5	35258	65863	6.80%	0.669%
38	17.051	2539	2544	2549	rBV8	13779	25760	2.66%	0.262%

Sum of corrected areas: 9848268

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101019\
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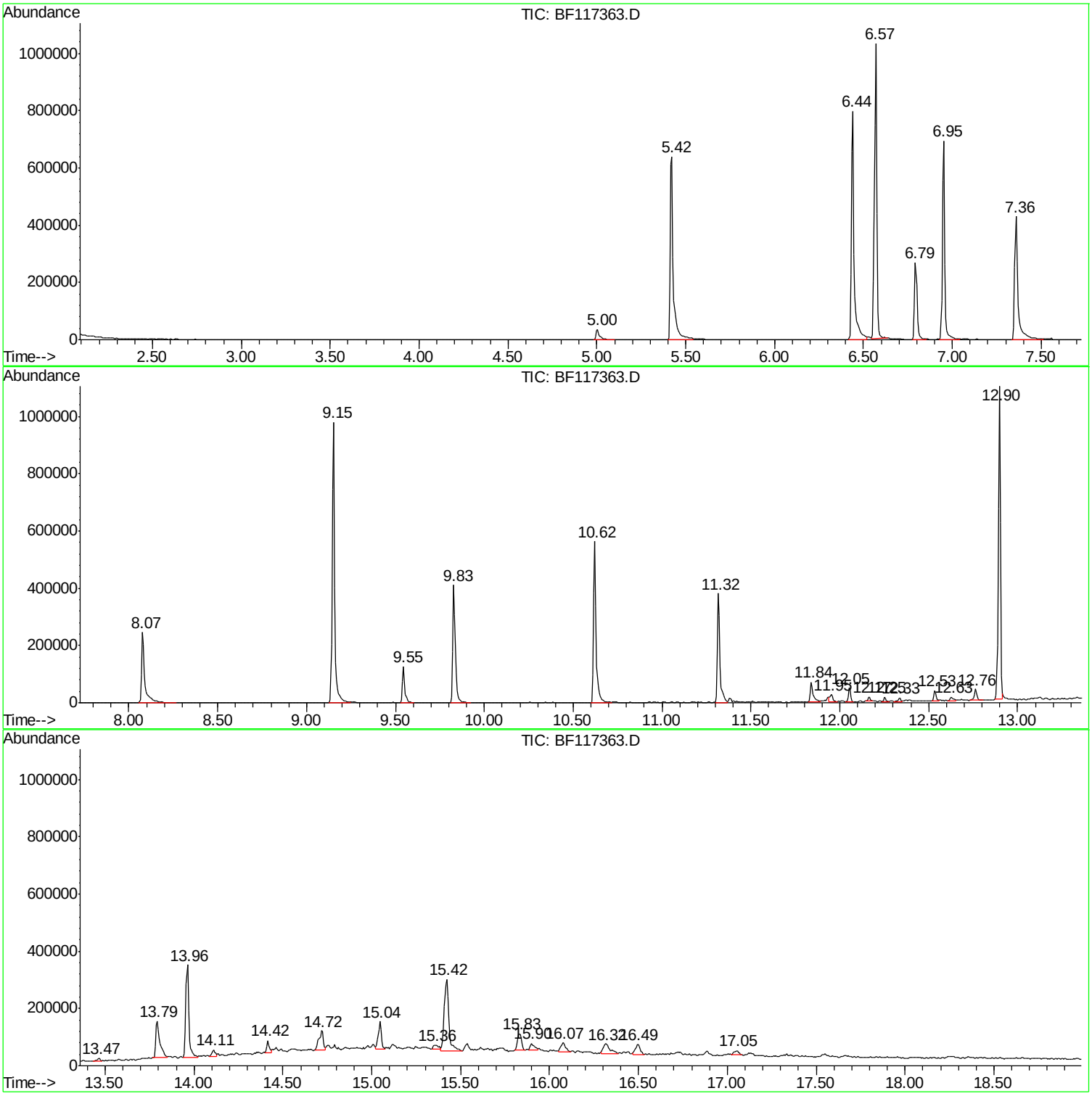
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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

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Data File : BF117363.D
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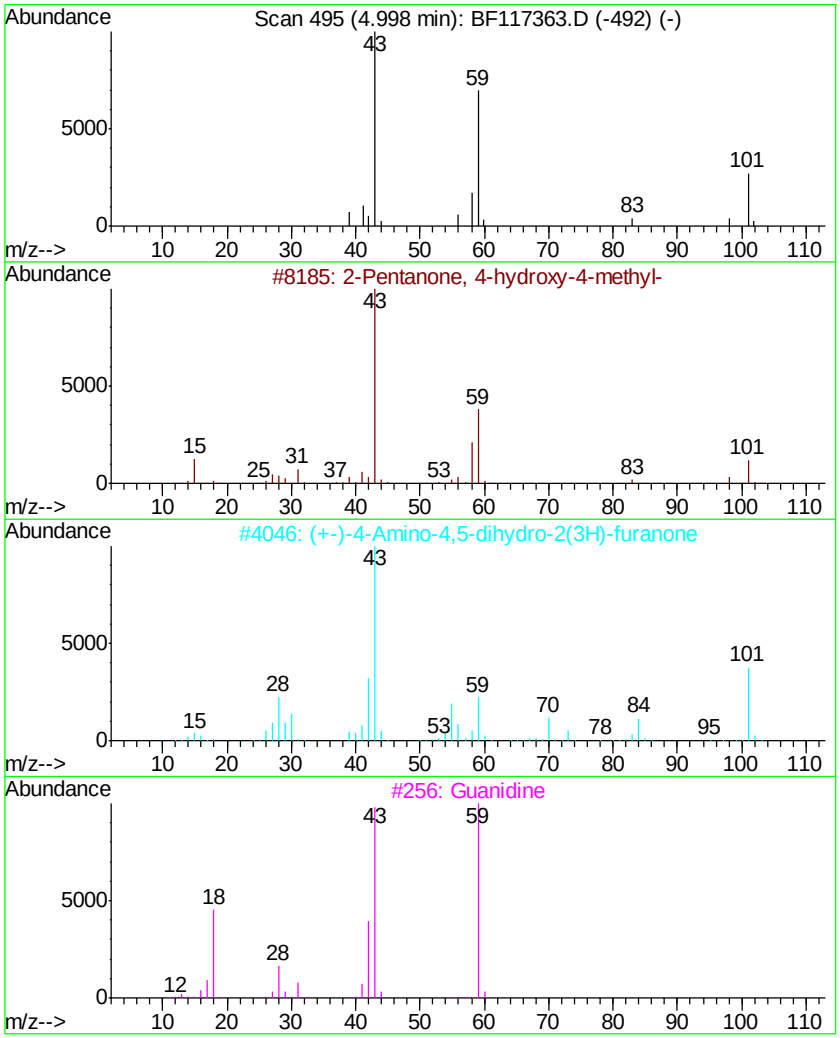
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

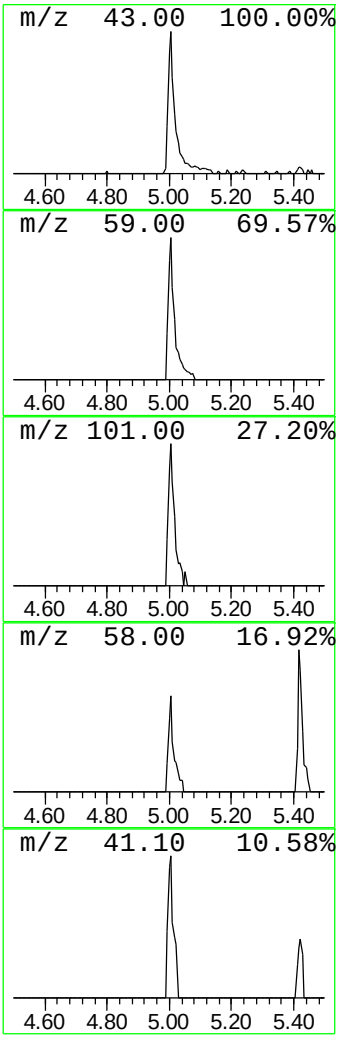
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	4.09 ng	51536	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
3	Guanidine	59	CH5N3	000113-00-8	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	2-Nonanone	142	C9H18O	000821-55-6	9





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Instrument :
BNA_F
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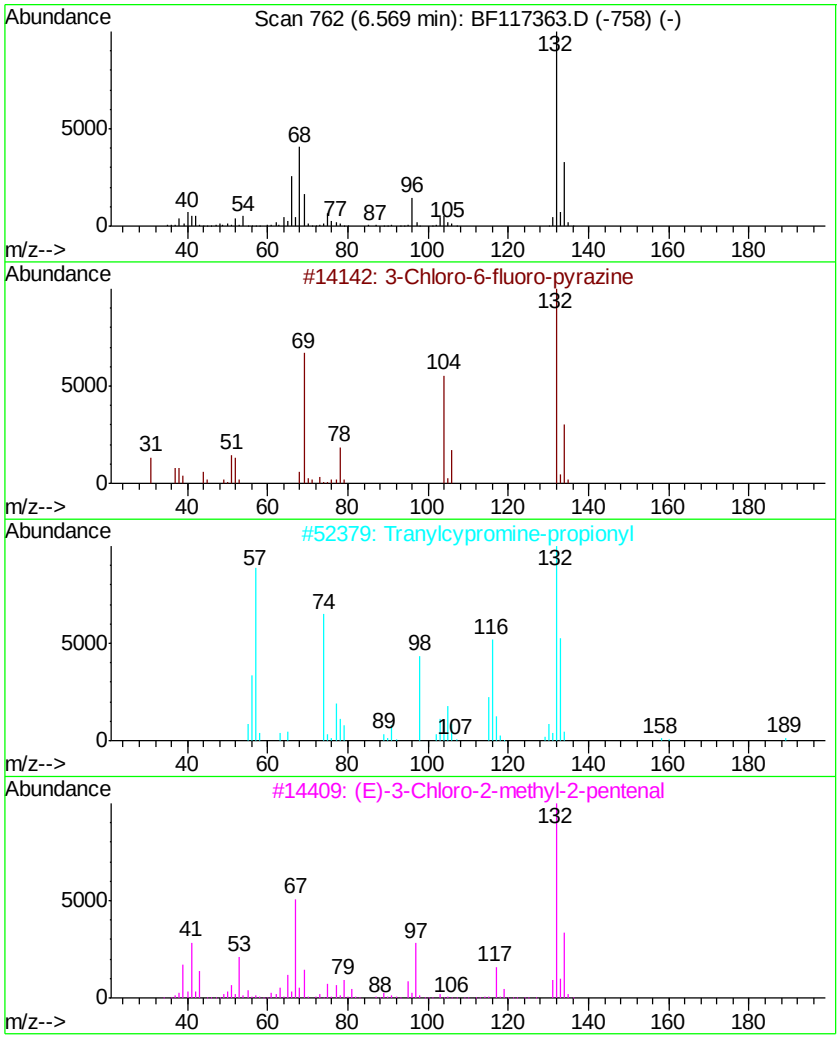
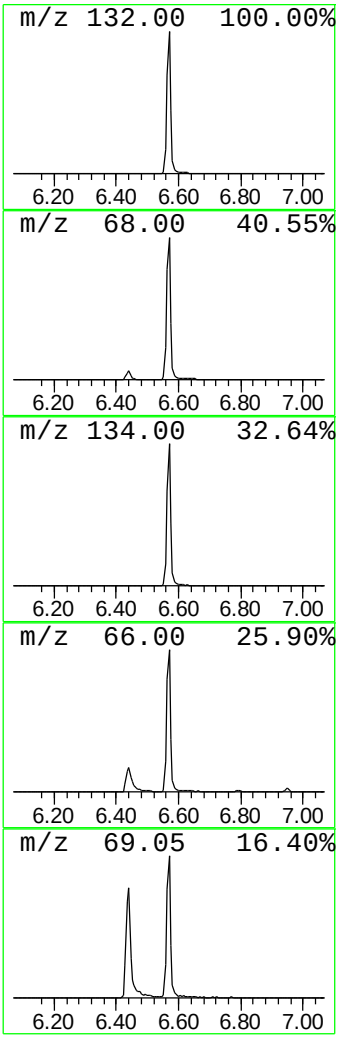
****

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	72.63 ng	914641	1,4-Dichlorobenzene-d4	6.79

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	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Library Search Compound Report

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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

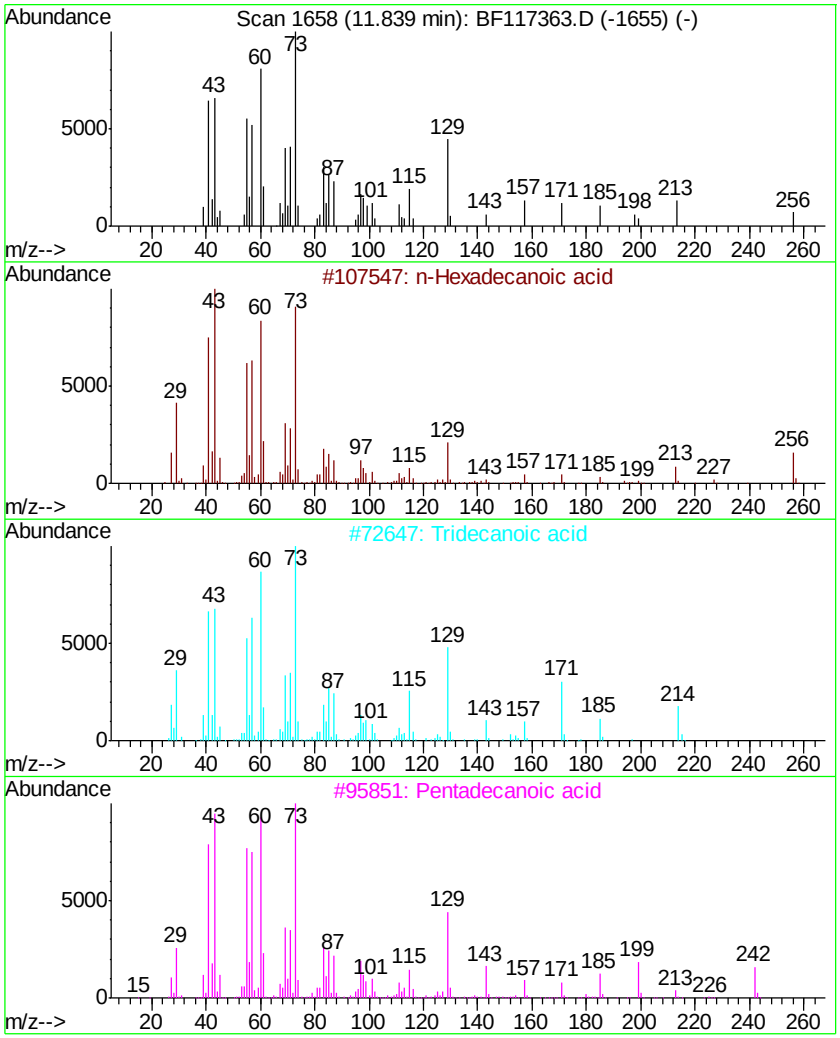
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

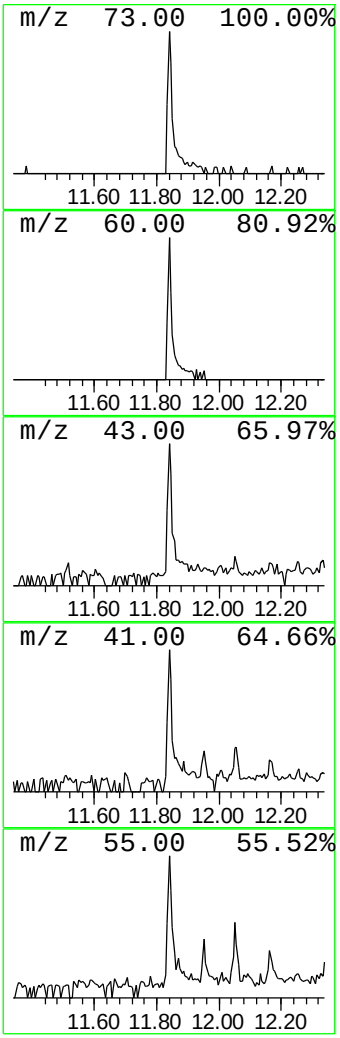
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	3.79 ng	76484	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	Tetradecane	198	C14H30	000629-59-4	15





Library Search Compound Report

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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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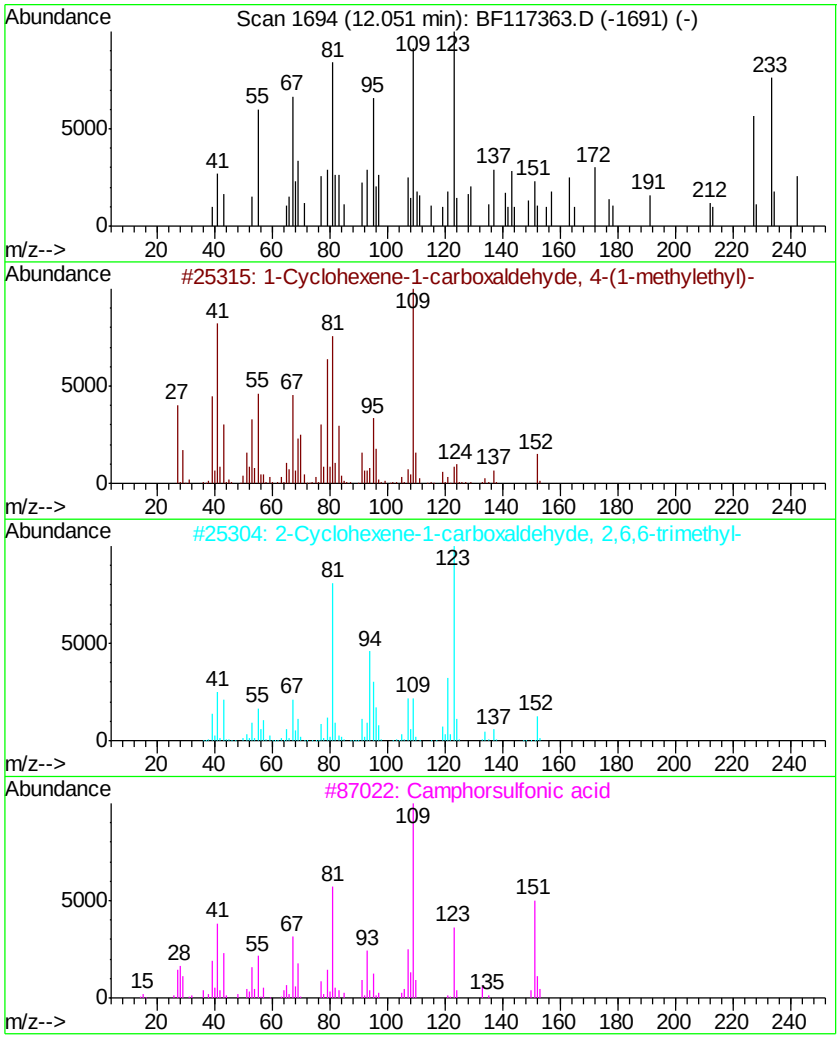
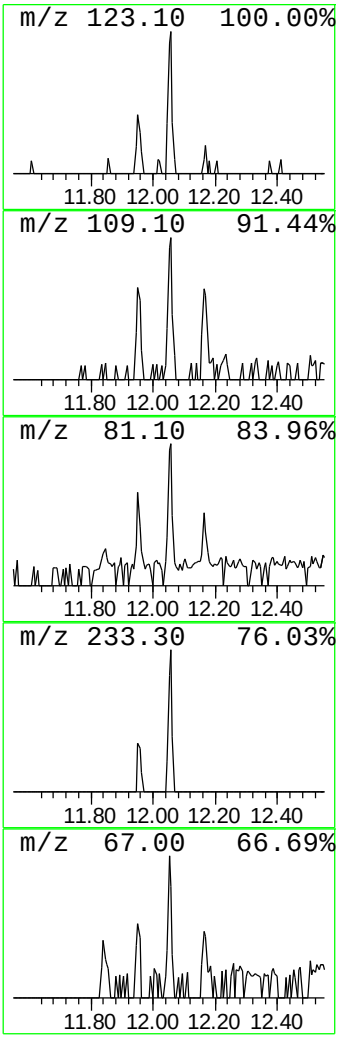
****

Peak Number 5 unknown12.05 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	2.23 ng	44985	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	021391-98-0	42
2	2-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	000432-24-6	30
3	Camphorsulfonic acid	232	C10H16O4S	003144-16-9	27
4	Bicyclo[2.2.1]heptane-1-methanes...	232	C10H16O4S	005872-08-2	27
5	trans-Chrysanthemol	154	C10H18O	018383-58-9	22





Library Search Compound Report

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Instrument :
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ClientSampleId :
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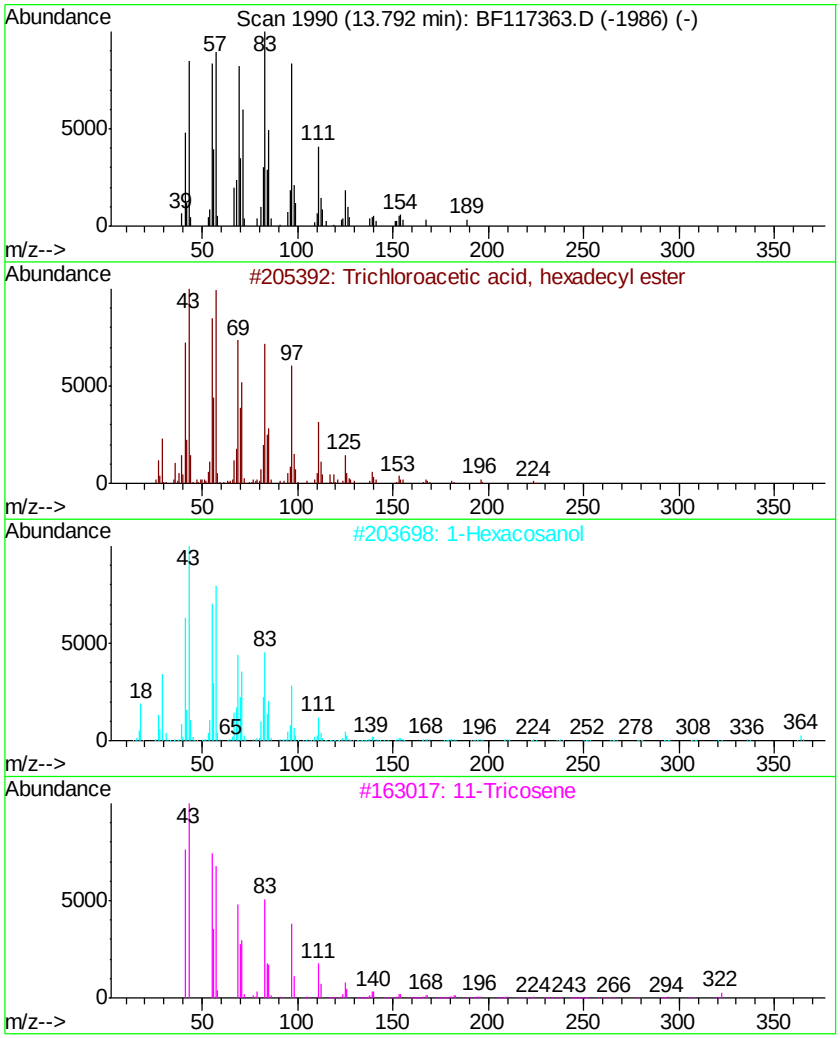
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

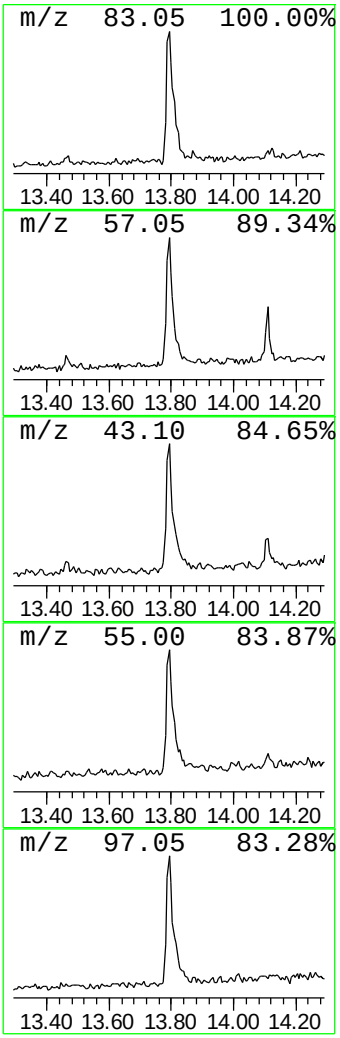
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	12.40 ng	215583	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2	1-Hexacosanol	382	C26H54O	000506-52-5	91
3	11-Tricosene	322	C23H46	052078-56-5	91
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	87





Library Search Compound Report

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

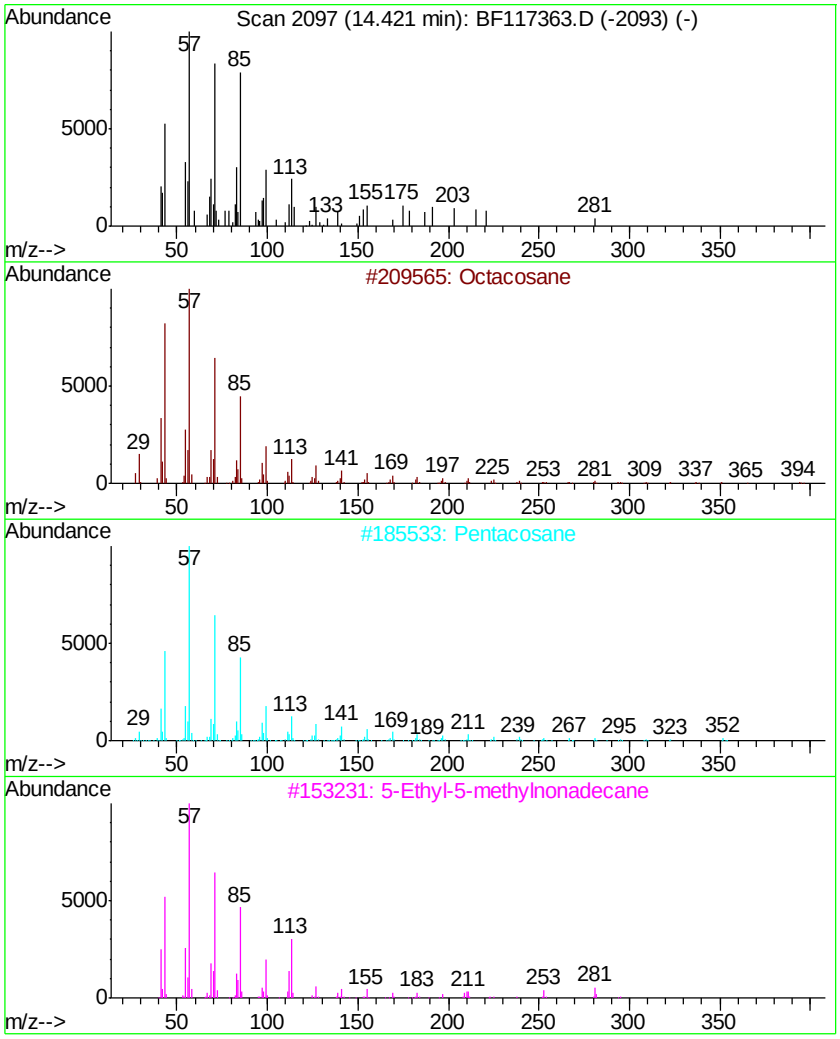
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

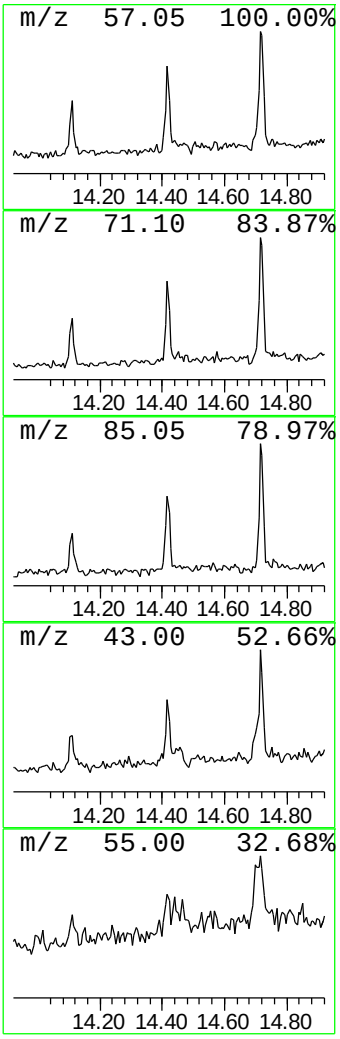
****

Peak Number 8 Octacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.42	2.38 ng	41437	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Pentacosane	352	C25H52	000629-99-2	86
3	5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	80
4	Heneicosane	296	C21H44	000629-94-7	72
5	Hexadecane	226	C16H34	000544-76-3	64





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

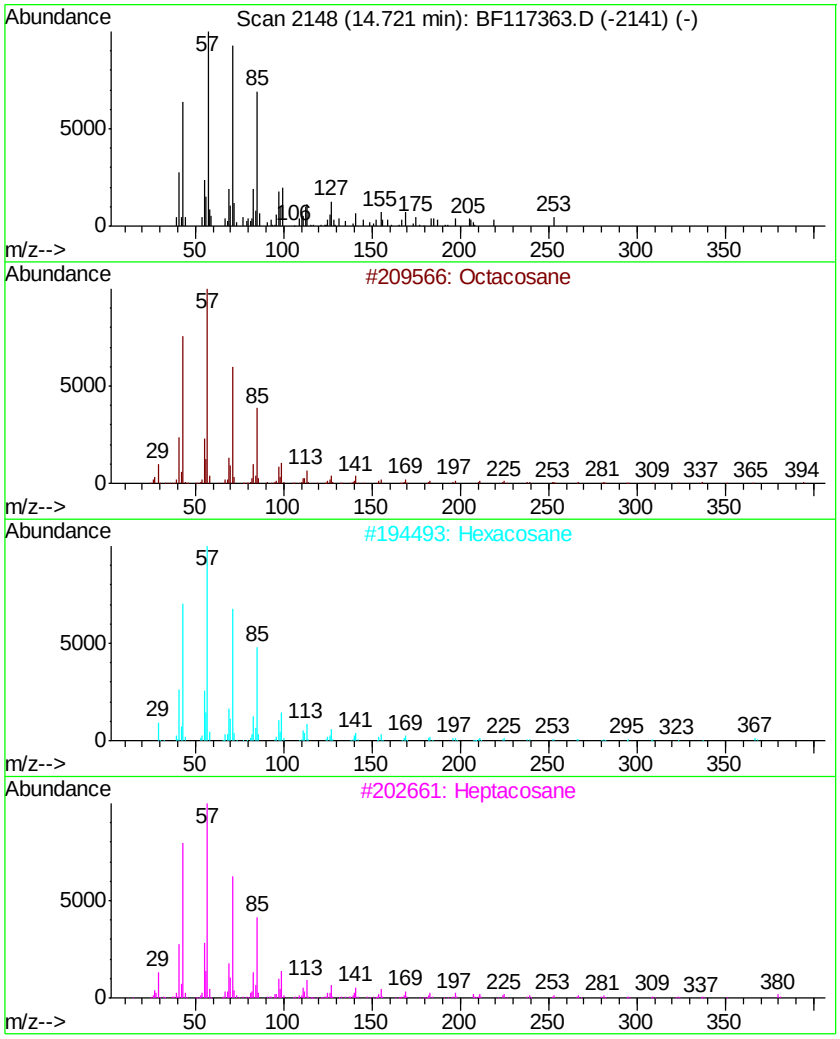
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

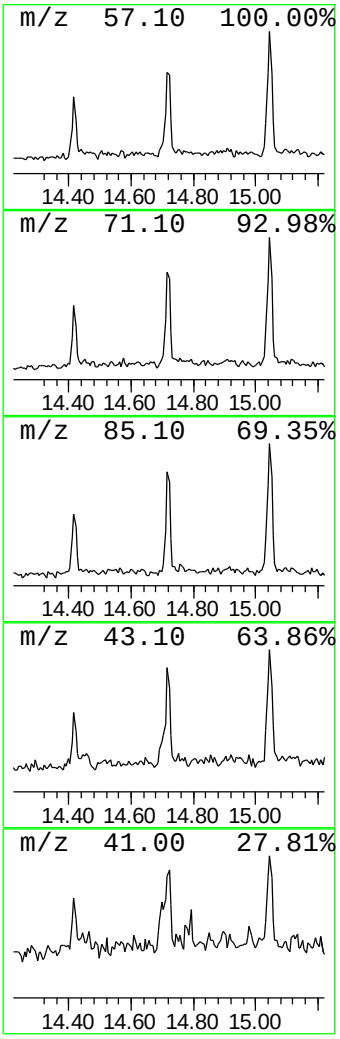
****

Peak Number 9 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	5.42 ng	116460	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Hexatriacontane	507	C36H74	000630-06-8	90
5	Heneicosane	296	C21H44	000629-94-7	87





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

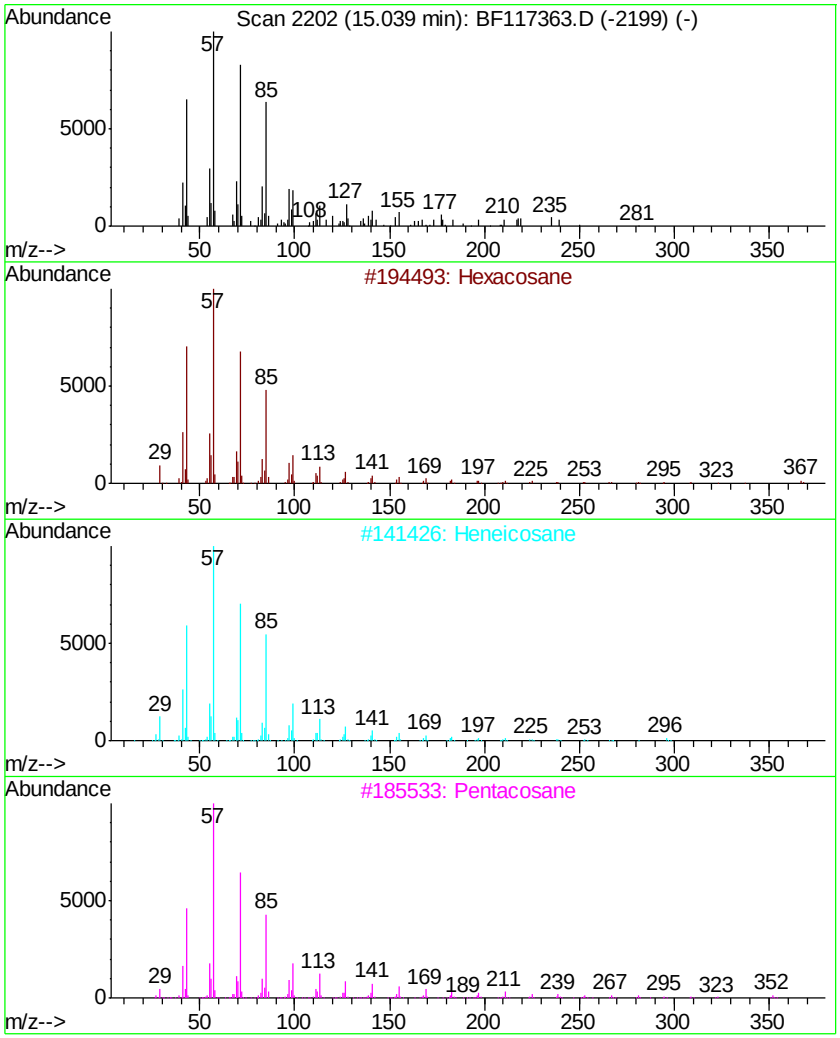
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

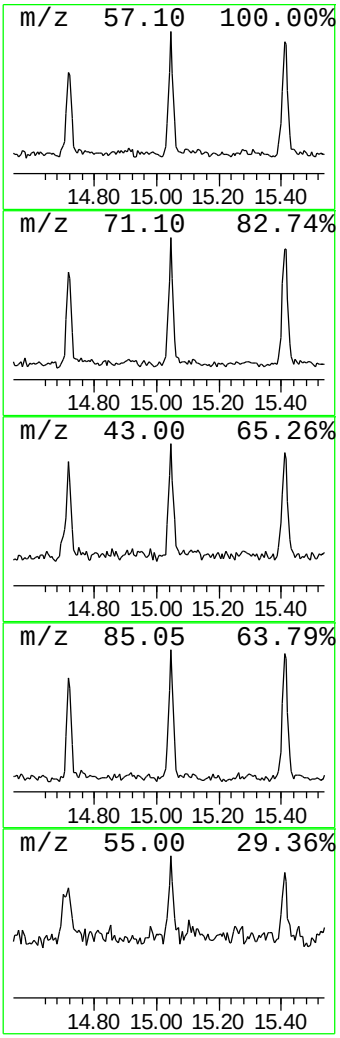
****

Peak Number 10 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	5.04 ng	108433	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Pentacosane	352	C25H52	000629-99-2	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Octacosane	394	C28H58	000630-02-4	91





Library Search Compound Report

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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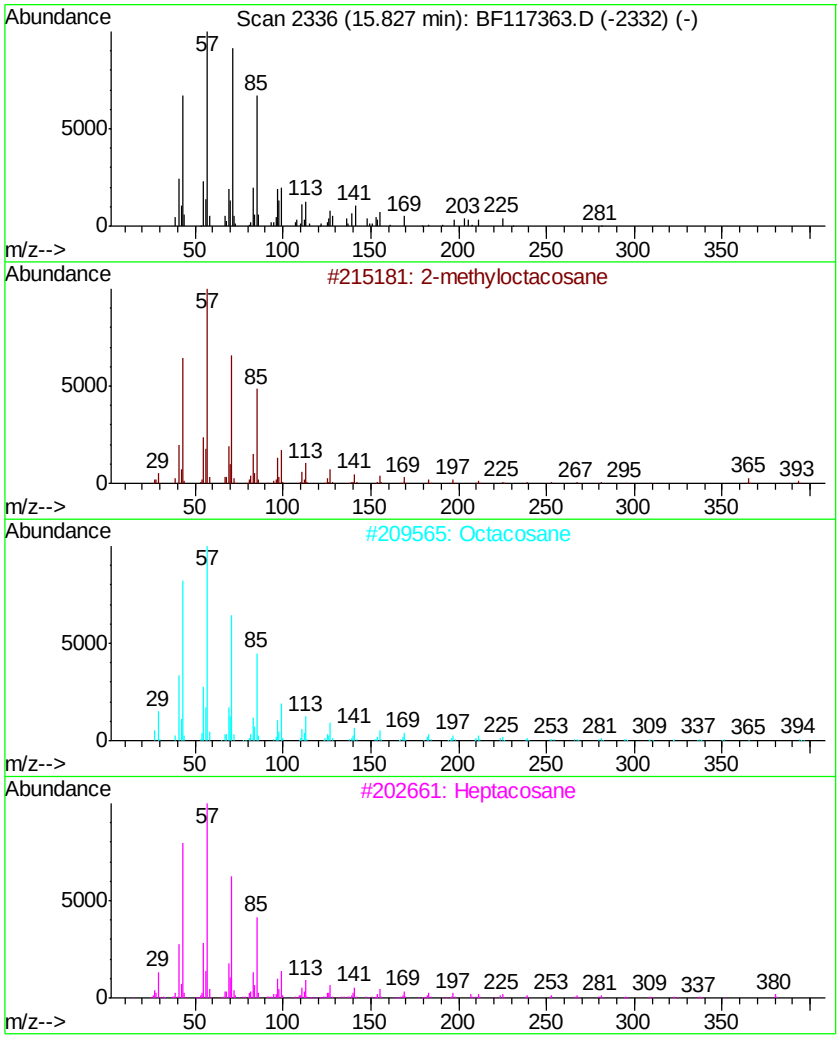
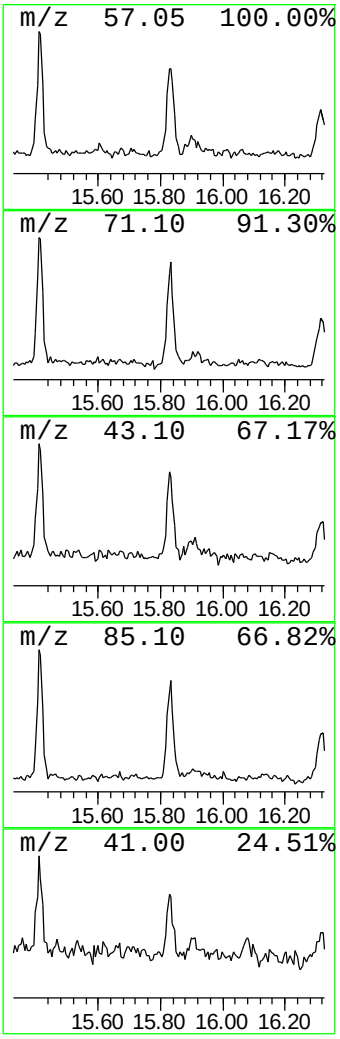
Peak Number 11 2-methyloctacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	3.92 ng	84260	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	86
2	Octacosane	394	C28H58	000630-02-4	86
3	Heptacosane	380	C27H56	000593-49-7	86
4	Hentriacontane	437	C31H64	000630-04-6	86
5	Hexacosane	366	C26H54	000630-01-3	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101019\
Data File : BF117363.D
Acq On : 10 Oct 2019 16:42
Operator : JU
Sample : K5297-14
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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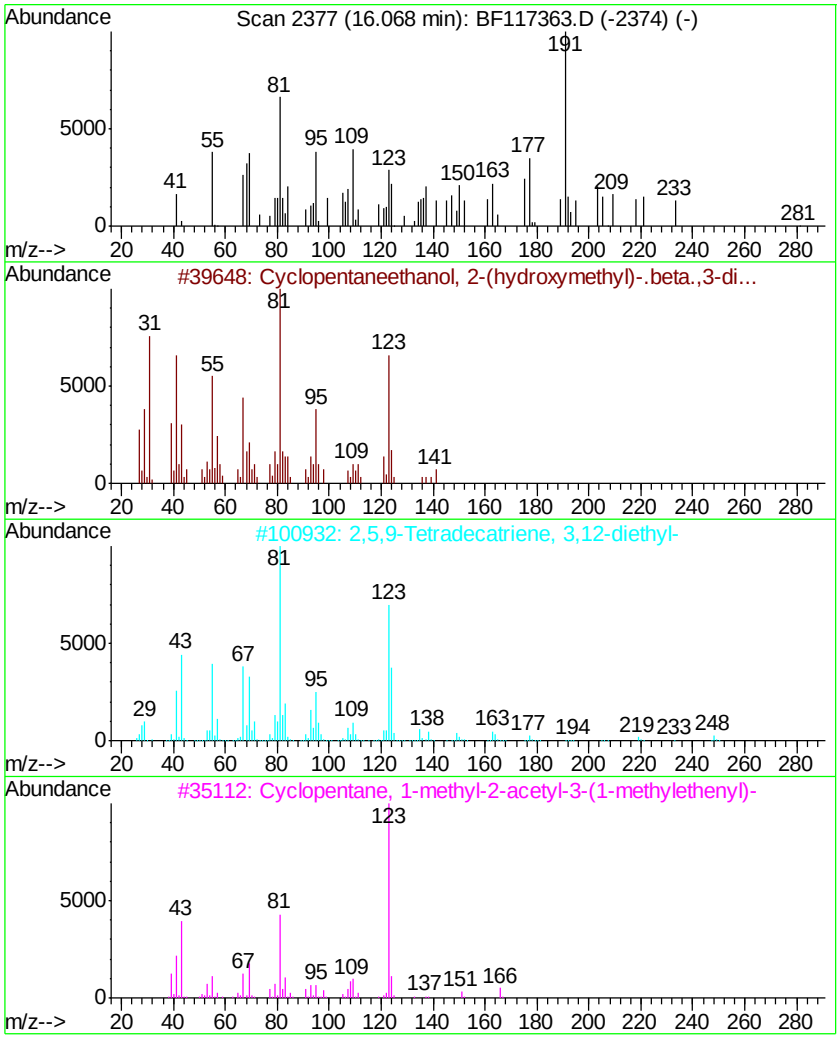
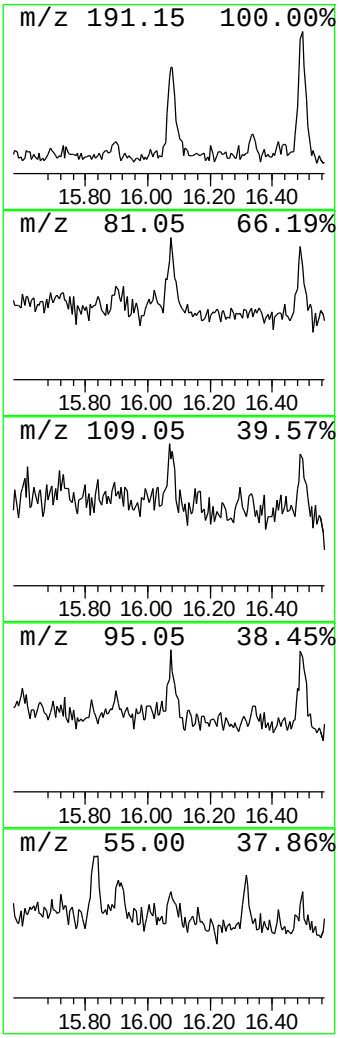
Peak Number 12 unknown16.07 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	2.92 ng	62841	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentaneethanol, 2-(hydroxym...	172	C10H20O2	000485-42-7	27
2	2,5,9-Tetradecatriene, 3,12-diet...	248	C18H32	074685-87-3	27
3	Cyclopentane, 1-methyl-2-acetyl-...	166	C11H18O	1000139-72-5	22
4	Bicyclo[3.3.1]nonan-9-one, 2,4-d...	211	C11H17NO3	129967-64-2	22
5	Naphthalene, 1-(1,1-dimethylethy...	194	C14H26	056292-64-9	22





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101019\
Data File : BF117363.D
Acq On : 10 Oct 2019 16:42
Operator : JU
Sample : K5297-14
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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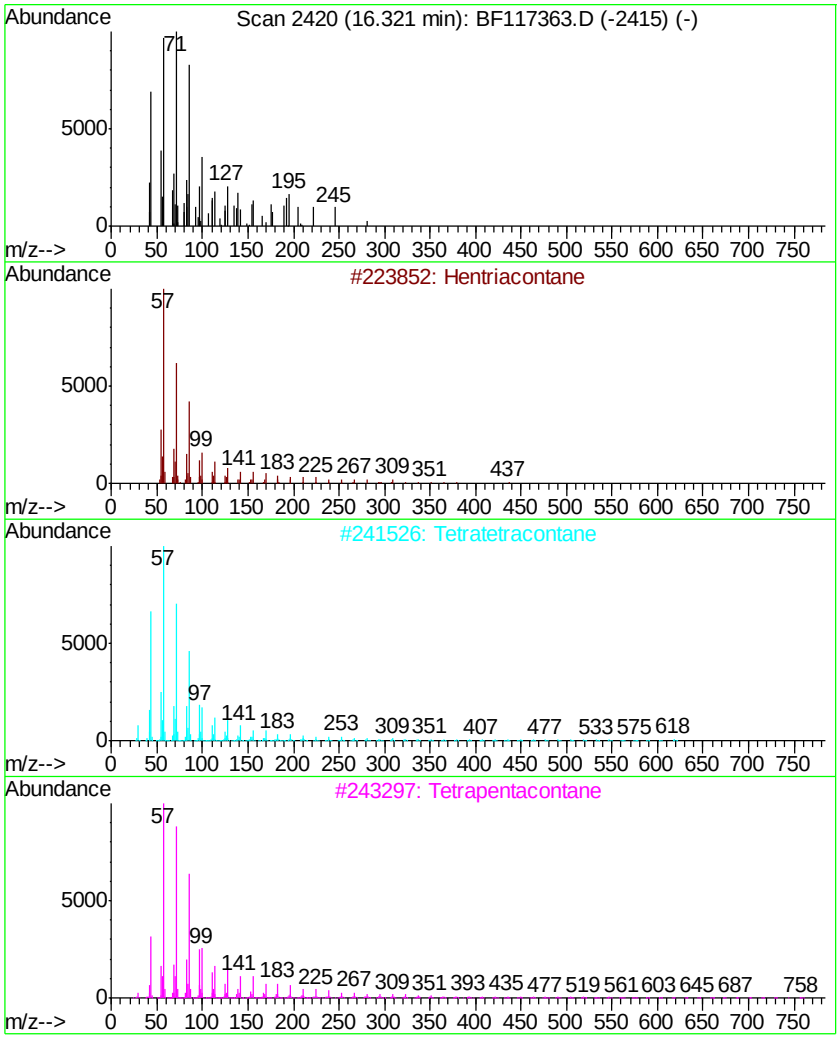
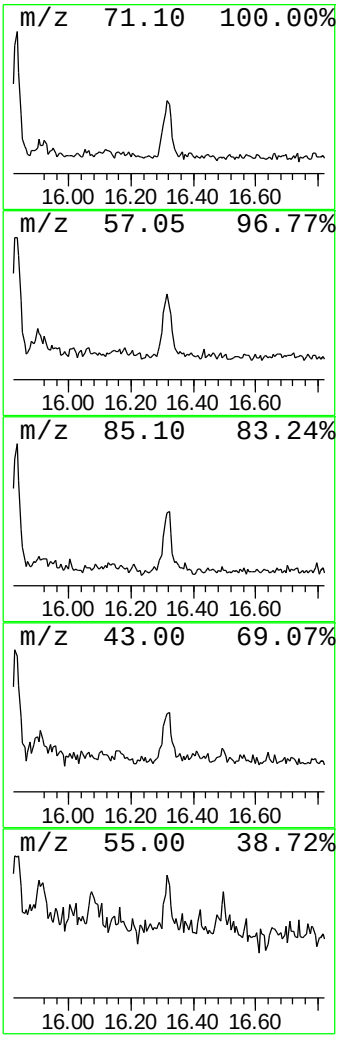
Peak Number 13 Hentriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.32	4.48 ng	96233	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	87
2	Tetratetracontane	619	C44H90	007098-22-8	86
3	Tetrapentacontane	759	C54H110	005856-66-6	86
4	Heptacosane	380	C27H56	000593-49-7	80
5	Methoxyacetic acid, 4-hexadecyl ...	314	C19H38O3	1000282-99-0	80





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101019\
Data File : BF117363.D
Acq On : 10 Oct 2019 16:42
Operator : JU
Sample : K5297-14
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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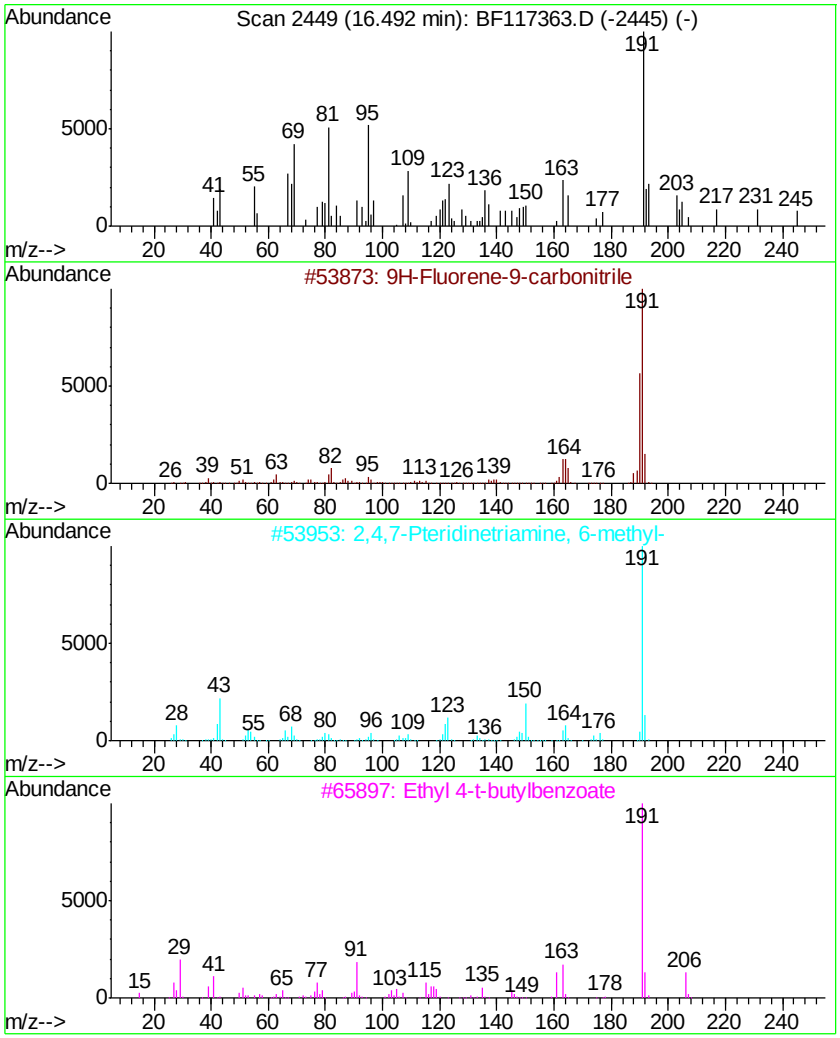
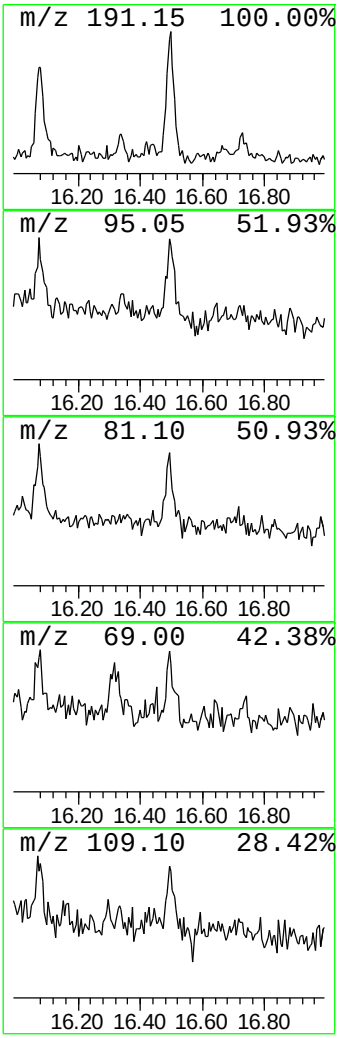
Peak Number 14 unknown16.49 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.49	3.06 ng	65863	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9H-Fluorene-9-carbonitrile	191	C14H9N	001529-40-4	43
2	2,4,7-Pteridinetriamine, 6-methyl-	191	C7H9N7	017539-50-3	35
3	Ethyl 4-t-butylbenzoate	206	C13H18O2	005406-57-5	35
4	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	27
5	Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101019\
Data File : BF117363.D
Acq On : 10 Oct 2019 16:42
Operator : JU
Sample : K5297-14
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	5.00	4.1	ng	51536	1	6.79	251855	20.0
unknown6.57	6.57	72.6	ng	914641	1	6.79	251855	20.0
n-Hexadecanoic acid	11.84	3.8	ng	76484	4	11.32	403911	20.0
unknown12.05	12.05	2.2	ng	44985	4	11.32	403911	20.0
Trichloroacetic a...	13.79	12.4	ng	215583	5	13.96	347742	20.0
Octacosane	14.42	2.4	ng	41437	5	13.96	347742	20.0
Hexacosane	14.72	5.4	ng	116460	6	15.42	430081	20.0
Heneicosane	15.04	5.0	ng	108433	6	15.42	430081	20.0
2-methyloctacosane	15.83	3.9	ng	84260	6	15.42	430081	20.0
unknown16.07	16.07	2.9	ng	62841	6	15.42	430081	20.0
Hentriacontane	16.32	4.5	ng	96233	6	15.42	430081	20.0
unknown16.49	16.49	3.1	ng	65863	6	15.42	430081	20.0