LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121619\
Data File : BF118219.D
Acq On : 17 Dec 2019 1:50
Operator : JU
Sample : K6284-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 42-SPRUCE

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-BF120619.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	5.063	502	506	514	rBV	297751	344550	13.90%	1.508%
2	5.475	572	576	591	rBV	1824969	1849587	74.61%	8.098%
3	6.416	732	736	742	rBV	33646	36478	1.47%	0.160%
4	6.493	745	749	766	rBV	2033966	2036597	82.15%	8.916%
5	6.634	769	773	776	rBV	2630649	2116516	85.37%	9.266%
6	6.863	808	812	820	rBV	622933	493887	19.92%	2.162%
7	7.022	835	839	842	rBV	1855716	1674400	67.54%	7.331%
8	7.428	903	908	919	rBV	1396997	1234612	49.80%	5.405%
9	8.151	1027	1031	1046	rBV	673656	633068	25.54%	2.772%
10	9.228	1210	1214	1217	rBV	3200141	2479143	100.00%	10.854%
11	9.622	1278	1281	1291	rBV	81742	74324	3.00%	0.325%
12	9.910	1326	1330	1343	rVB	893621	734024	29.61%	3.214%
13	10.704	1461	1465	1481	rBV	1762904	1605103	64.74%	7.027%
14	11.404	1580	1584	1586	rBV	838019	688246	27.76%	3.013%
15	11.428	1586	1588	1593	rVB	160224	135717	5.47%	0.594%
16	11.910	1666	1670	1671	rBV	52889	55098	2.22%	0.241%
17	11.928	1671	1673	1681	rVV3	185548	228881	9.23%	1.002%
18	12.016	1685	1688	1691	rVV2	66400	77908	3.14%	0.341%
19	12.045	1691	1693	1699	rVB	44608	42911	1.73%	0.188%
20	12.233	1723	1725	1730	rVB	34976	34326	1.38%	0.150%
21	12.457	1760	1763	1766	rBV	41307	43541	1.76%	0.191%
22	12.622	1786	1791	1796	rBV	239364	223698	9.02%	0.979%
23	12.716	1804	1807	1811	rBV3	59205	55418	2.24%	0.243%
24	12.810	1820	1823	1826	rBV2	38601	44193	1.78%	0.193%
25	12.851	1826	1830	1837	rVB	257468	259656	10.47%	1.137%
26	12.992	1850	1854	1858	rBV	2510175	2182484	88.03%	9.555%
27	13.074	1864	1868	1872	rBV4	31435	46439	1.87%	0.203%
28	13.286	1901	1904	1907	rBV	41537	35316	1.42%	0.155%
29	13.380	1917	1920	1923	rBV	36587	33294	1.34%	0.146%
30	13.692	1968	1973	1977	rBV	37481	47051	1.90%	0.206%
31	13.804	1987	1992	1995	rBV2	43395	57295	2.31%	0.251%
32	13.886	2003	2006	2017	rVB2	240474	321781	12.98%	1.409%
33	14.057	2029	2035	2038	rBV2	696277	798805	32.22%	3.497%
34	14.080	2038	2039	2045	rVB	154668	111980	4.52%	0.490%

LSC Area Percent Report

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Operator : JU
Sample : K6284-01
Misc :
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Instrument : BNA_F
ClientSampleId : 42-SPRUCE

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-BF120619.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.210	2057	2061	2068	rBV5	55722	78736	3.18%	0.345%
36	14.445	2099	2101	2104	rVB	43376	34203	1.38%	0.150%
37	14.516	2110	2113	2120	rBV4	68673	92227	3.72%	0.404%
38	14.827	2164	2166	2169	rBV2	33410	31846	1.28%	0.139%
39	14.904	2176	2179	2183	rVB3	25819	32378	1.31%	0.142%
40	15.110	2210	2214	2217	rBV	106018	158980	6.41%	0.696%
41	15.168	2221	2224	2229	rVB	95081	104086	4.20%	0.456%
42	15.416	2262	2266	2273	rVB	77186	116038	4.68%	0.508%
43	15.480	2273	2277	2283	rVB	94523	121383	4.90%	0.531%
44	15.545	2283	2288	2304	rBV	580433	875833	35.33%	3.834%
45	16.004	2362	2366	2371	rVB	80172	116709	4.71%	0.511%
46	16.063	2372	2376	2382	rVB6	35672	68217	2.75%	0.299%
47	17.051	2539	2544	2551	rVB2	37753	77922	3.14%	0.341%
48	17.233	2570	2575	2577	rBV6	18605	36251	1.46%	0.159%
49	17.504	2616	2621	2627	rBV2	28028	59845	2.41%	0.262%

Sum of corrected areas: 22840981

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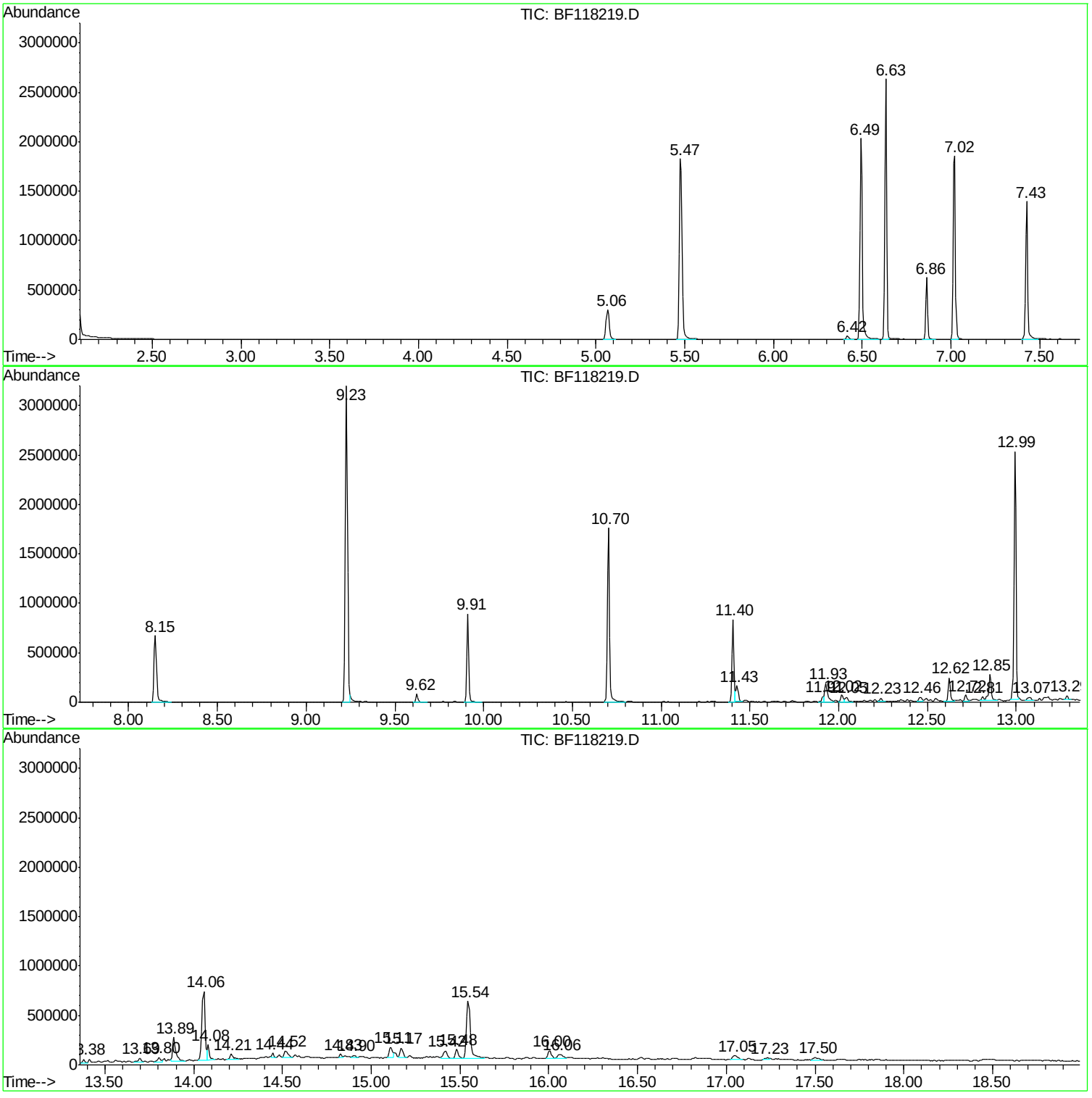
Instrument :
BNA_F
ClientSampleId :
42-SPRUCE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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 : BF118219.D
Acq On : 17 Dec 2019 1:50
Operator : JU
Sample : K6284-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 42-SPRUCE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

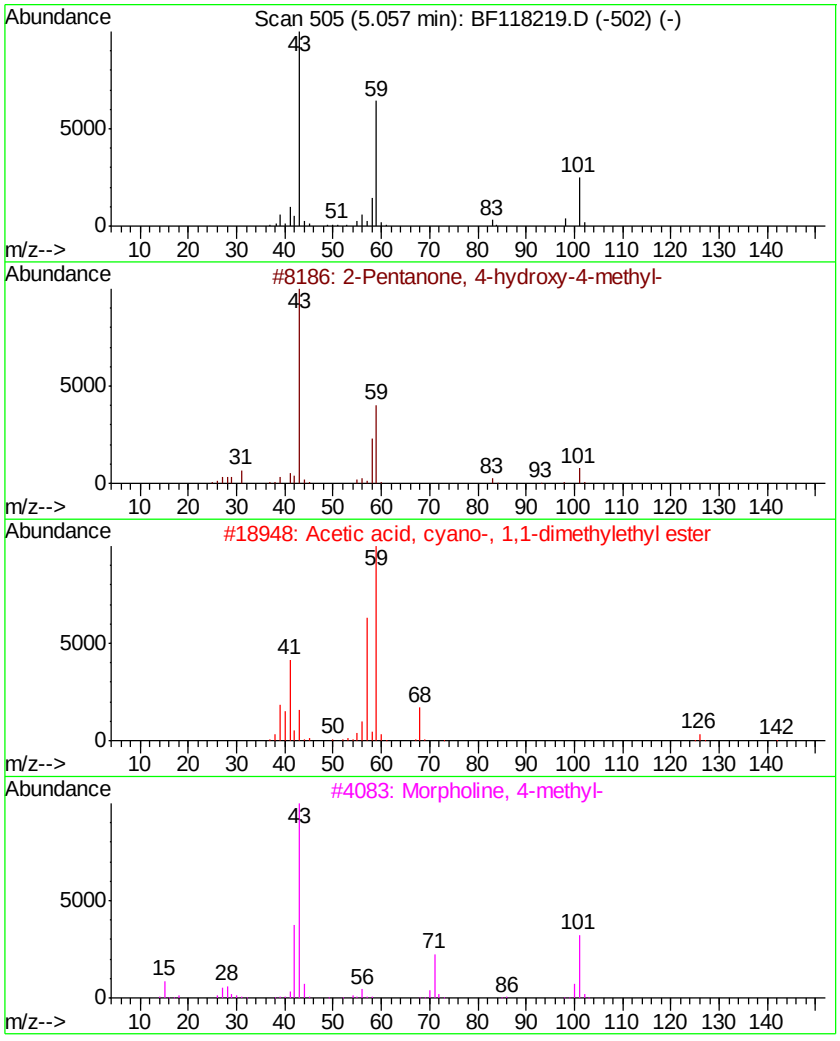
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

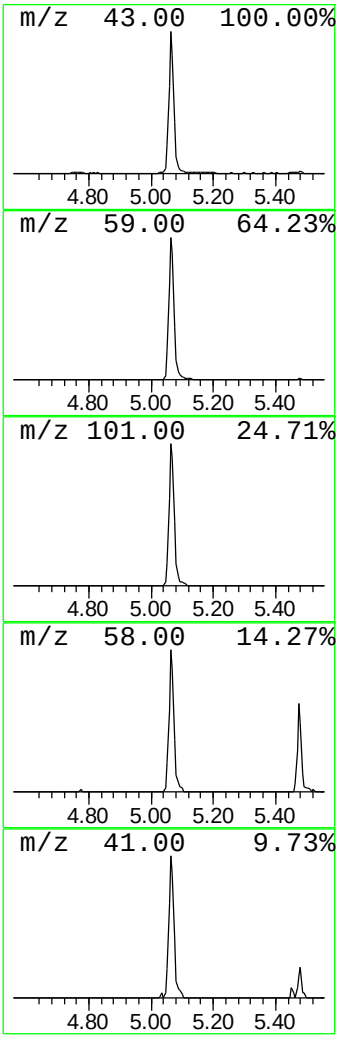
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	13.95 ng	344550	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Misc :
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Instrument : BNA_F
ClientSampleId : 42-SPRUCE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

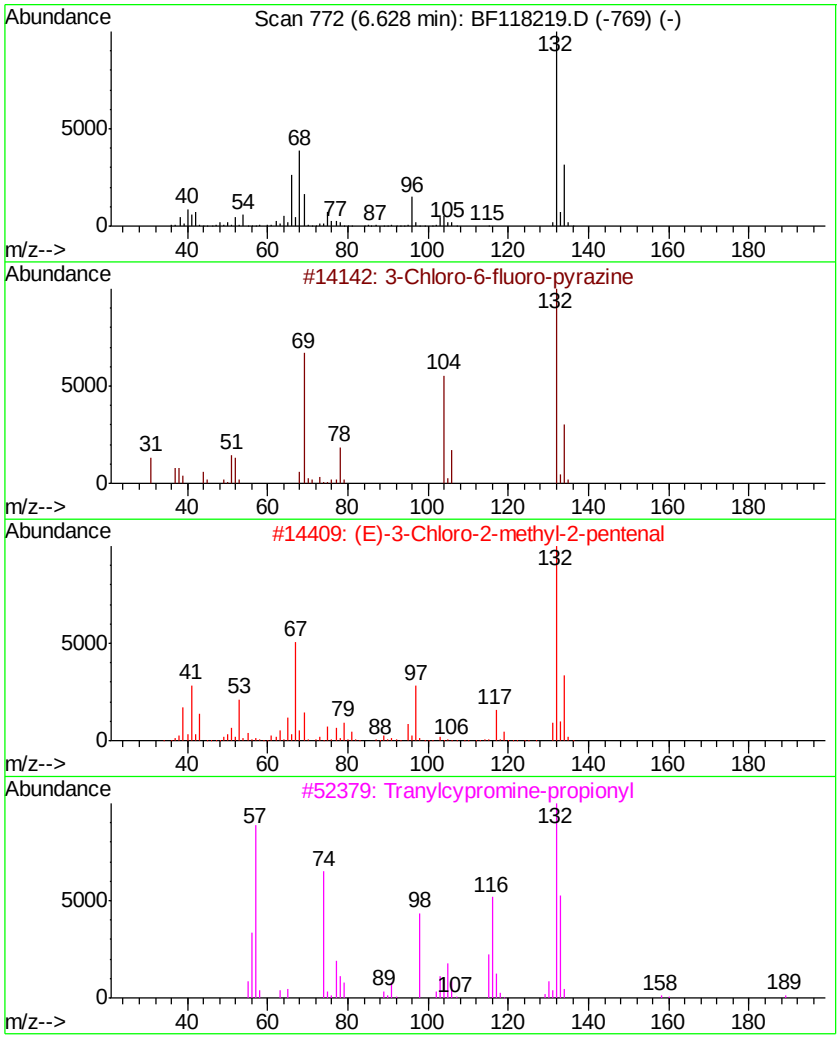
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

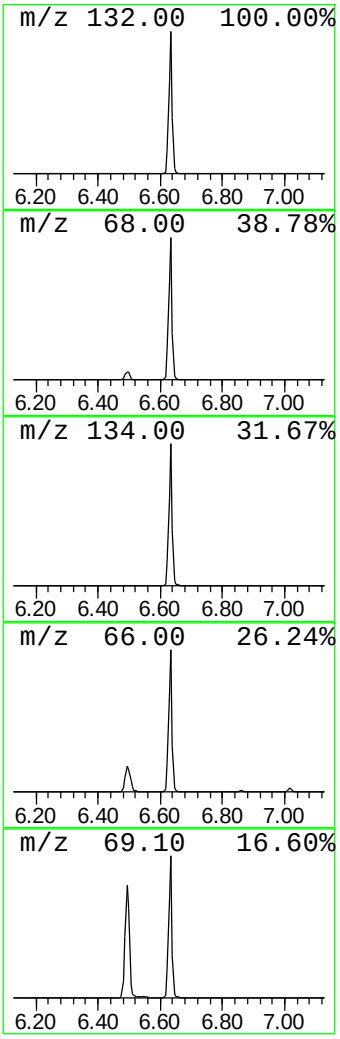
****

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	85.71 ng	2116520	1,4-Dichlorobenzene-d4	6.86

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	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4	5-Aminoindole	132	C8H8N2	005192-03-0	16
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

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Acq On : 17 Dec 2019 1:50
Operator : JU
Sample : K6284-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 42-SPRUCE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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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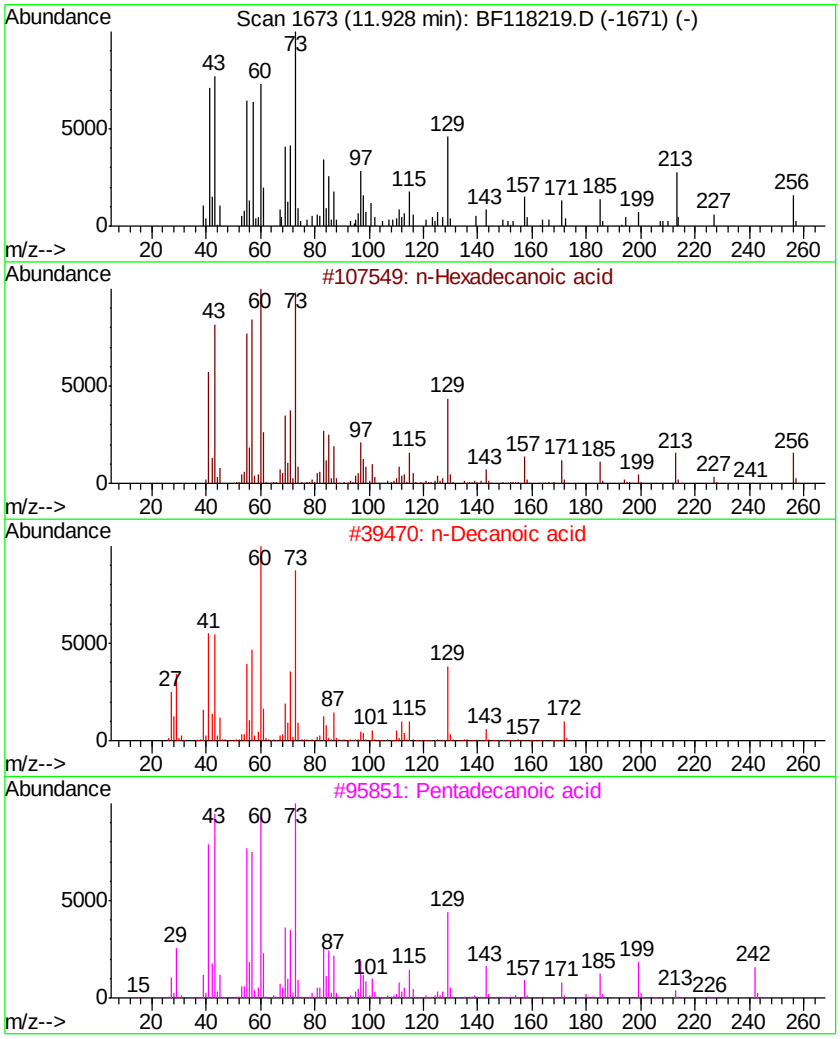
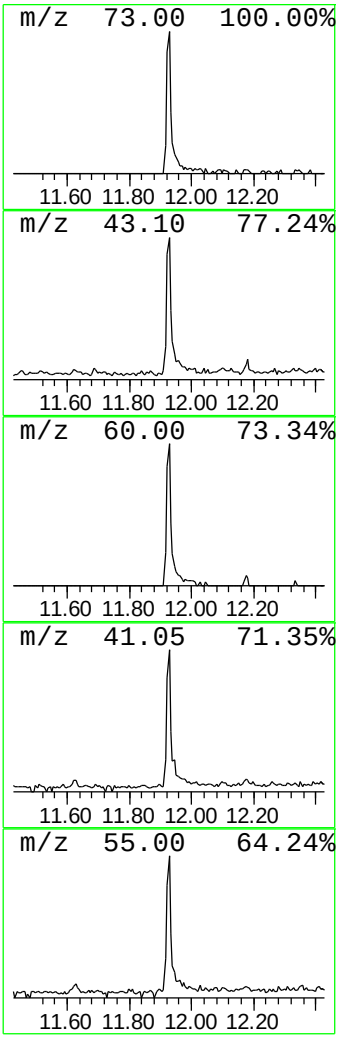
Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	6.65 ng	228881	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	n-Decanoic acid	172	C10H20O2	000334-48-5	70
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	3,7-Dimethyl-8-oxo-1,5-dioxa-spi...	256	C13H20O5	1000193-79-8	25





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Operator : JU
Sample : K6284-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 42-SPRUCE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

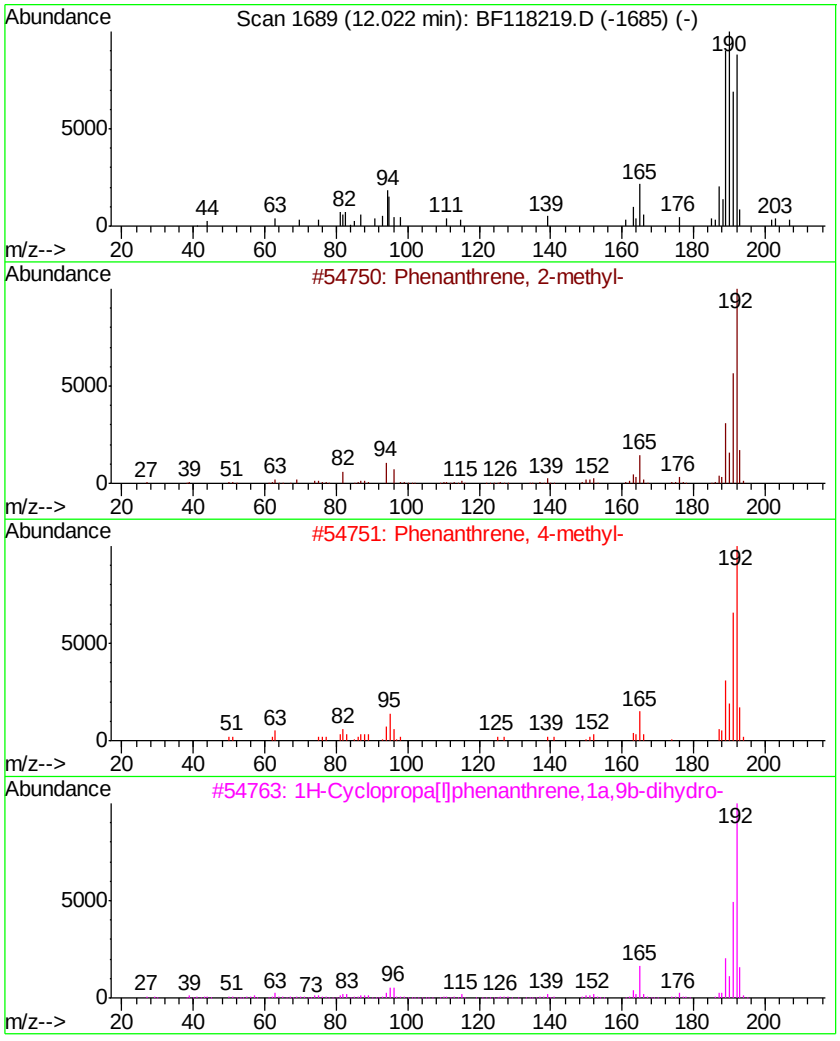
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

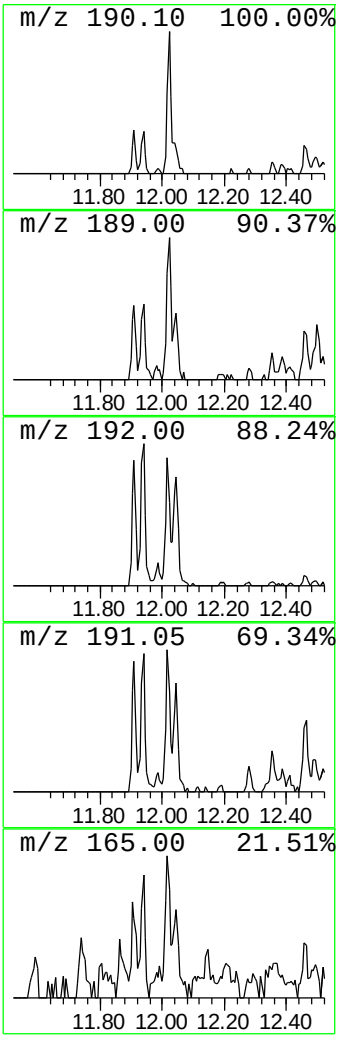
****

Peak Number 5 Phenanthrene, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	2.26 ng	77908	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	60
3	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	60
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	60
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	60





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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 42-SPRUCE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

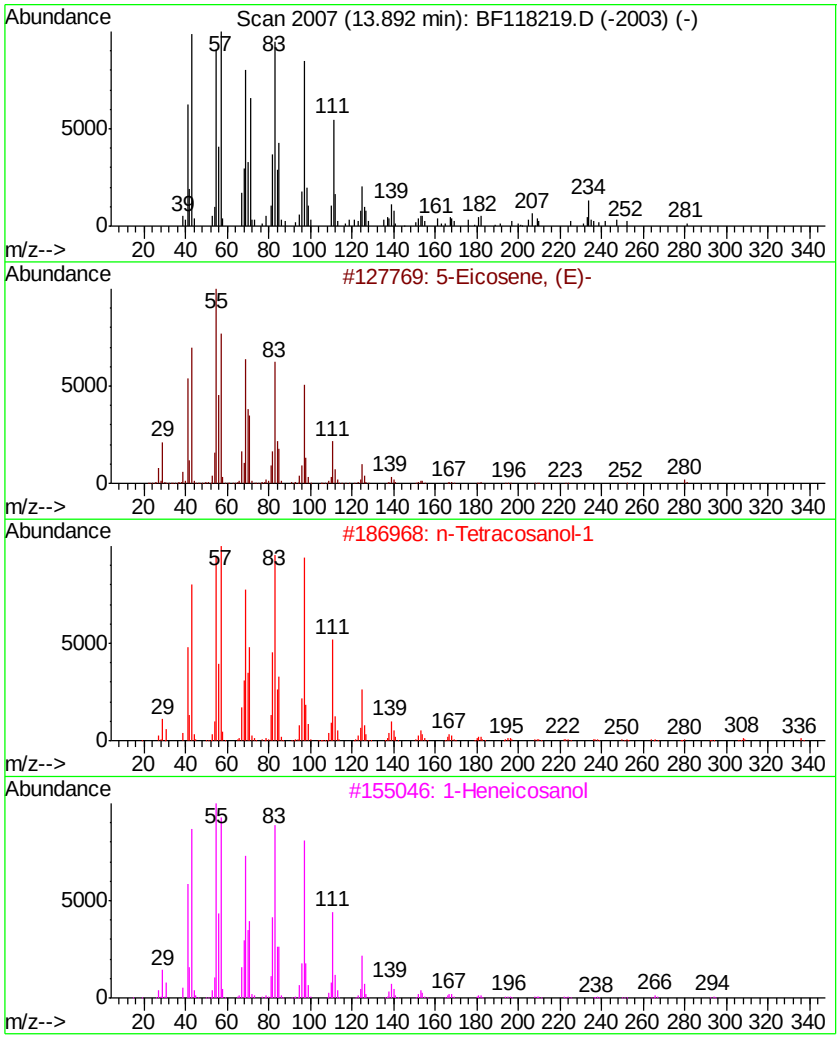
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

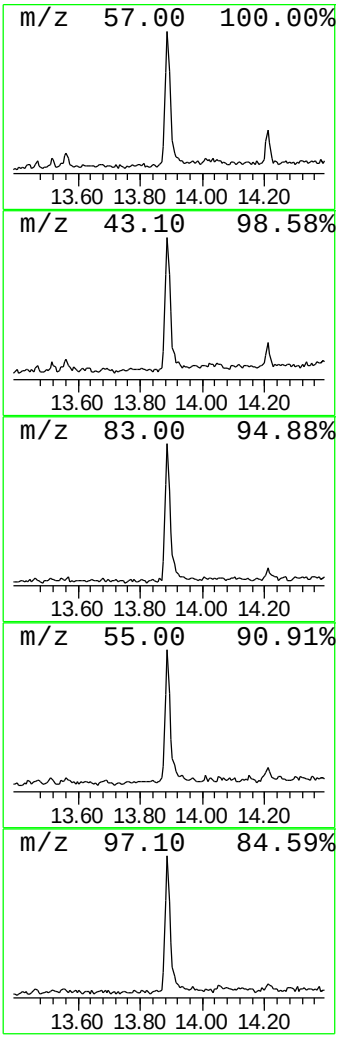
****

Peak Number 6 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	8.06 ng	321781	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	Behenic alcohol	326	C22H46O	000661-19-8	95
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	95





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Data File : BF118219.D
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Instrument : BNA_F
ClientSampleId : 42-SPRUCE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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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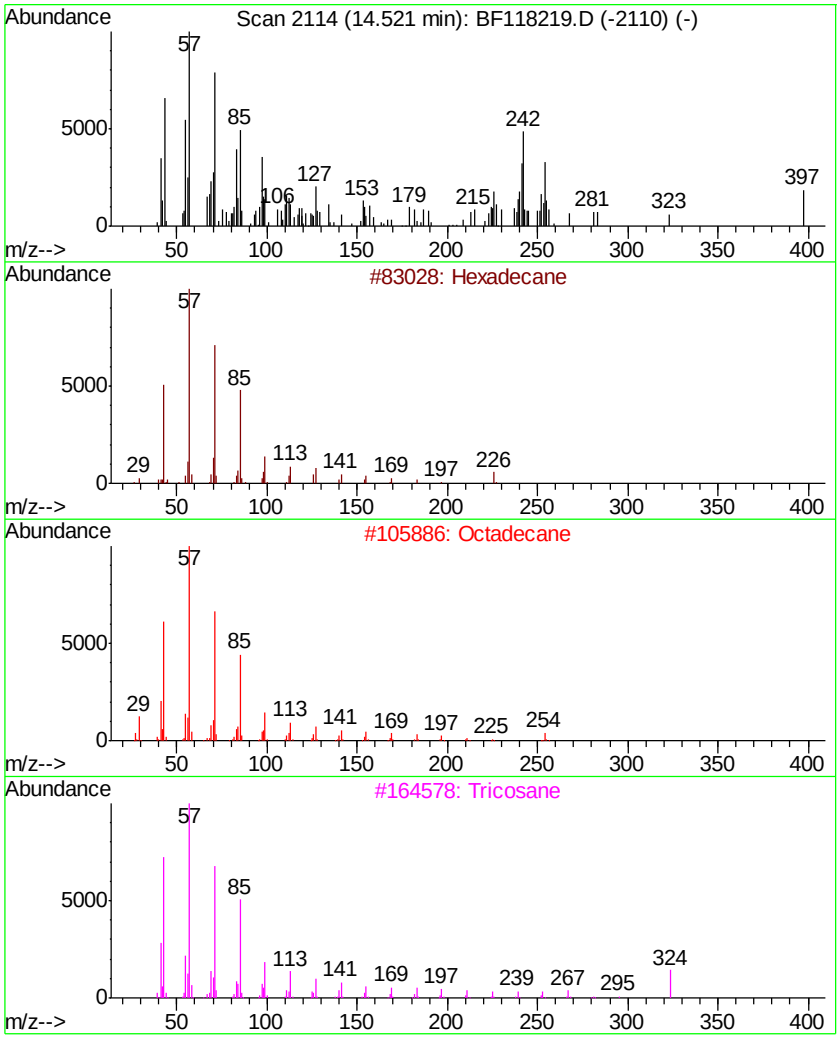
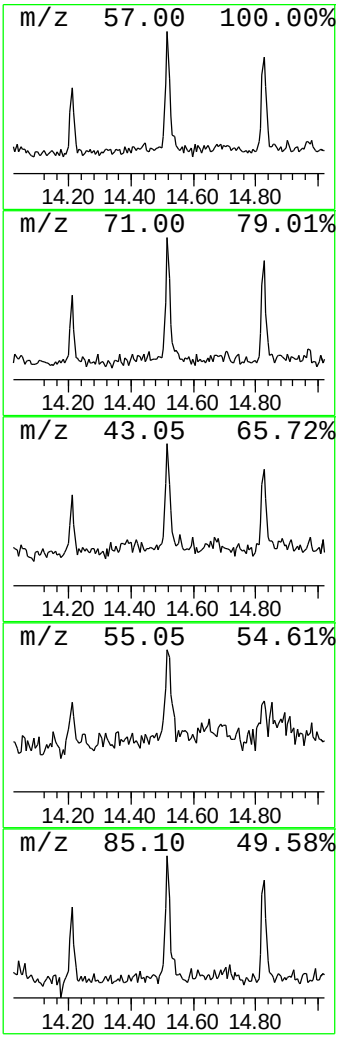
Peak Number 7 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	2.31 ng	92227	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	70
2	Octadecane	254	C18H38	000593-45-3	60
3	Tricosane	324	C23H48	000638-67-5	53
4	Nonadecane	268	C19H40	000629-92-5	53
5	Heptadecane	240	C17H36	000629-78-7	52





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Instrument : BNA_F
ClientSampleId : 42-SPRUCE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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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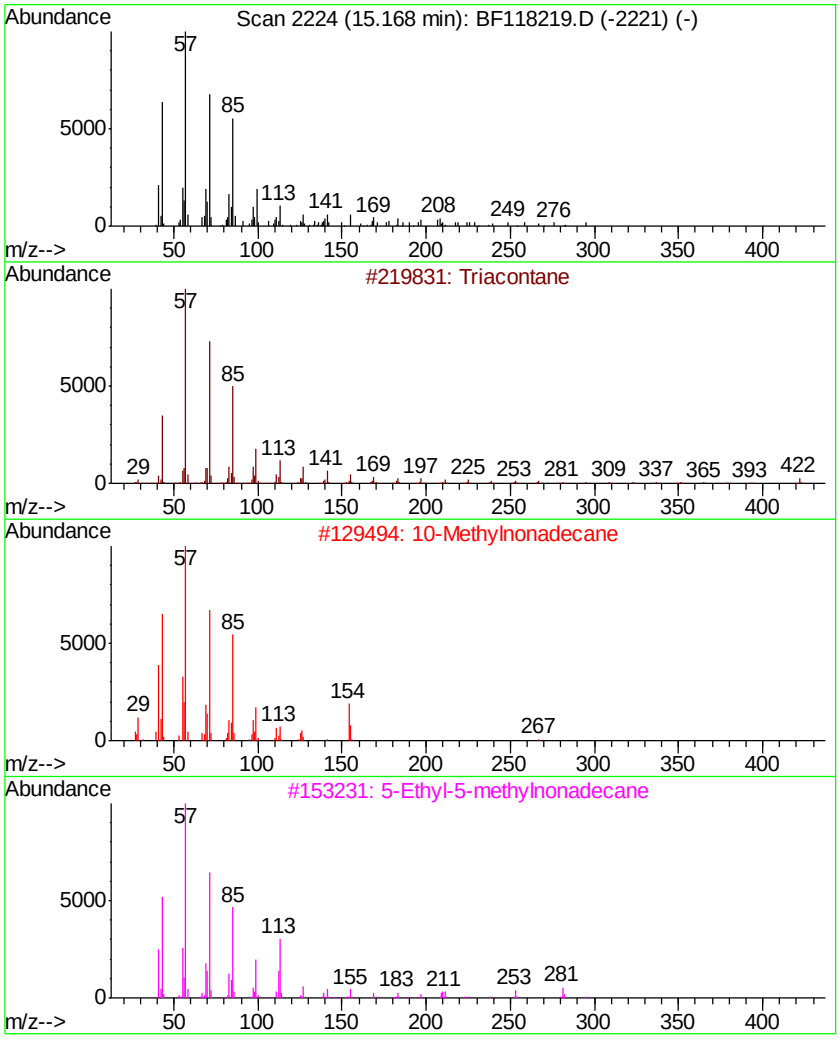
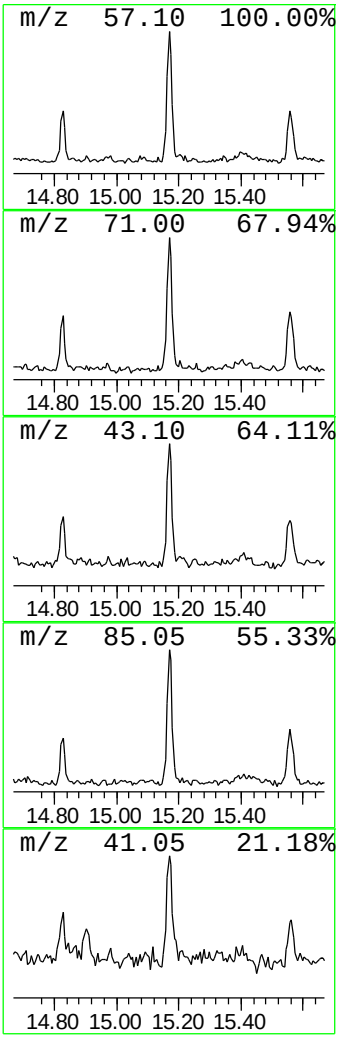
Peak Number 8 Triacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	2.38 ng	104086	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	87
2	10-Methylnonadecane	282	C20H42	056862-62-5	86
3	5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	83
4	Hexadecane	226	C16H34	000544-76-3	81
5	Octacosane	394	C28H58	000630-02-4	80





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121619\
Data File : BF118219.D
Acq On : 17 Dec 2019 1:50
Operator : JU
Sample : K6284-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 42-SPRUCE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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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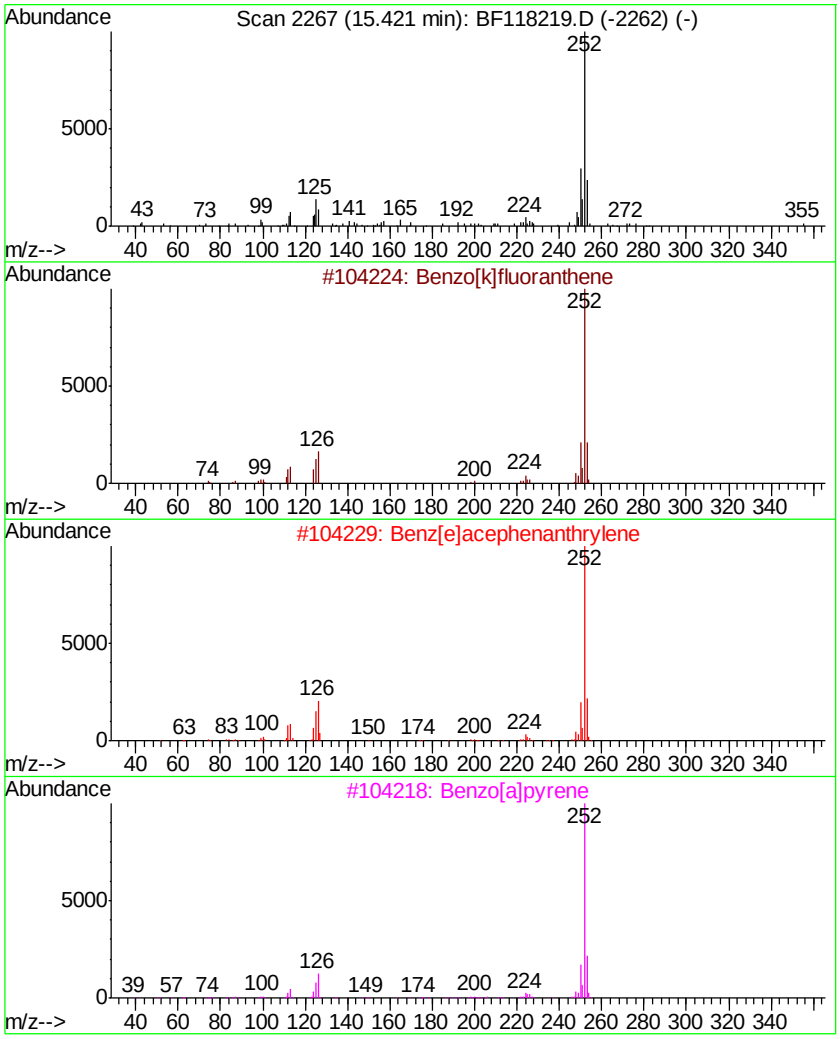
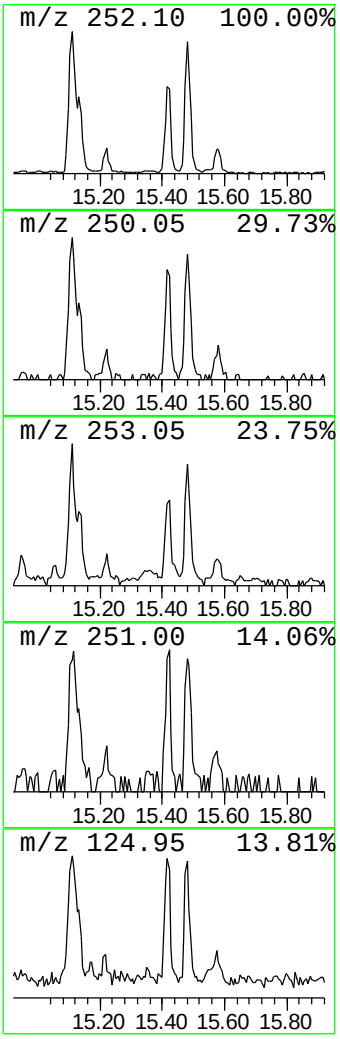
Peak Number 9 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.42	2.65 ng	116038	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	90
3	Benzo[a]pyrene	252	C20H12	000050-32-8	87
4	Benzo[e]pyrene	252	C20H12	000192-97-2	87
5	Perylene	252	C20H12	000198-55-0	76





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121619\
Data File : BF118219.D
Acq On : 17 Dec 2019 1:50
Operator : JU
Sample : K6284-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 42-SPRUCE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

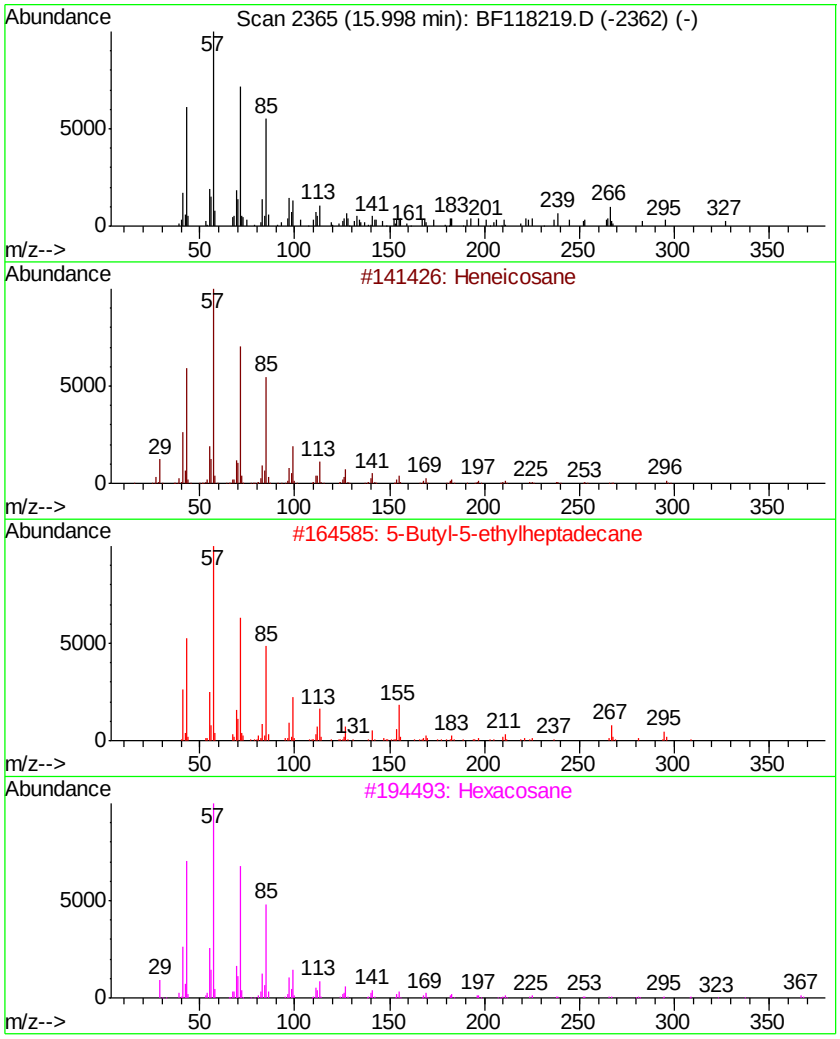
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

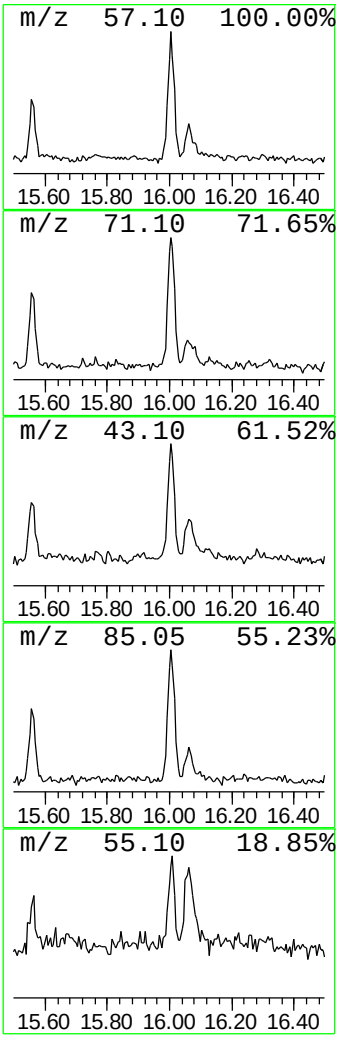
****

Peak Number 10 5-Butyl-5-ethylheptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.00	2.67 ng	116709	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	99
2	5-Butyl-5-ethylheptadecane	324	C23H48	1000360-43-0	86
3	Hexacosane	366	C26H54	000630-01-3	83
4	Tricosane, 2-methyl-	338	C24H50	001928-30-9	80
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121619\
Data File : BF118219.D
Acq On : 17 Dec 2019 1:50
Operator : JU
Sample : K6284-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 42-SPRUCE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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
2-Pentanone, 4-hy...	5.06	13.9	ng	344550	1	6.86	493887	20.0
unknown6.63	6.63	85.7	ng	2116520	1	6.86	493887	20.0
n-Hexadecanoic acid	11.93	6.7	ng	228881	4	11.40	688246	20.0
Phenanthrene, 2-m...	12.02	2.3	ng	77908	4	11.40	688246	20.0
5-Eicosene, (E)-	13.89	8.1	ng	321781	5	14.06	798805	20.0
Hexadecane	14.52	2.3	ng	92227	5	14.06	798805	20.0
Triacontane	15.17	2.4	ng	104086	6	15.54	875833	20.0
Benzo[e]pyrene	15.42	2.6	ng	116038	6	15.54	875833	20.0
5-Butyl-5-ethylhe...	16.00	2.7	ng	116709	6	15.54	875833	20.0