LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118344.D
Acq On : 27 Dec 2019 18:11
Operator : JU
Sample : K6431-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4-(0-2)

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-BF122419.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	5.057	501	505	517	rVB	430069	535253	14.89%	1.356%
2	5.469	571	575	591	rBV	2839665	2652294	73.76%	6.720%
3	6.487	743	748	758	rBV	2940278	2856452	79.44%	7.238%
4	6.622	767	771	774	rBV	3682000	3061078	85.13%	7.756%
5	6.851	806	810	817	rBV	1059737	870339	24.20%	2.205%
6	7.010	832	837	840	rBV	2652033	2418380	67.26%	6.128%
7	7.416	902	906	909	rBV	1983076	1749670	48.66%	4.433%
8	8.139	1025	1029	1045	rBV	1224848	1170041	32.54%	2.965%
9	9.216	1207	1212	1215	rBV	4341150	3595798	100.00%	9.111%
10	9.610	1276	1279	1288	rVB	462803	370651	10.31%	0.939%
11	9.898	1324	1328	1332	rBV	1660626	1363431	37.92%	3.455%
12	10.692	1459	1463	1479	rBV	2827598	2502230	69.59%	6.340%
13	11.392	1578	1582	1584	rBV	1652110	1383035	38.46%	3.504%
14	11.416	1584	1586	1591	rVV	729363	591864	16.46%	1.500%
15	11.469	1591	1595	1598	rVB	96721	93569	2.60%	0.237%
16	11.627	1616	1622	1628	rBV2	58369	94962	2.64%	0.241%
17	11.916	1668	1671	1679	rVB2	476735	514605	14.31%	1.304%
18	12.010	1683	1687	1689	rVV2	135868	145474	4.05%	0.369%
19	12.027	1689	1690	1694	rVB	62554	55343	1.54%	0.140%
20	12.192	1715	1718	1721	rBV	74933	63008	1.75%	0.160%
21	12.222	1721	1723	1729	rVB	99927	97271	2.71%	0.246%
22	12.445	1757	1761	1764	rBV	66682	69531	1.93%	0.176%
23	12.480	1764	1767	1770	rVV3	46331	56535	1.57%	0.143%
24	12.539	1773	1777	1781	rBV2	69555	80187	2.23%	0.203%
25	12.610	1785	1789	1794	rBV	1199215	1068149	29.71%	2.706%
26	12.704	1802	1805	1809	rBV2	116459	127727	3.55%	0.324%
27	12.763	1811	1815	1817	rVB3	38350	48786	1.36%	0.124%
28	12.845	1823	1829	1832	rBV	854892	974074	27.09%	2.468%
29	12.892	1835	1837	1842	rVB2	47397	50868	1.41%	0.129%
30	12.980	1845	1852	1856	rBV	3733604	3512617	97.69%	8.900%
31	13.057	1861	1865	1866	rBV	57689	64108	1.78%	0.162%
32	13.151	1877	1881	1882	rBV3	56817	70697	1.97%	0.179%
33	13.169	1882	1884	1888	rVB	84108	91404	2.54%	0.232%
34	13.239	1893	1896	1898	rVV	60868	52338	1.46%	0.133%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118344.D
Acq On : 27 Dec 2019 18:11
Operator : JU
Sample : K6431-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4-(0-2)

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-BF122419.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.274	1898	1902	1909	rVB2	86611	122038	3.39%	0.309%
36	13.398	1921	1923	1926	rBV2	48021	51881	1.44%	0.131%
37	13.551	1943	1949	1951	rBV3	64076	94187	2.62%	0.239%
38	13.686	1969	1972	1976	rVB	95217	82993	2.31%	0.210%
39	13.792	1987	1990	1993	rBV	86575	93579	2.60%	0.237%
40	13.821	1993	1995	1997	rVB	61008	45129	1.26%	0.114%
41	13.845	1997	1999	2000	rBV	56205	45509	1.27%	0.115%
42	13.874	2000	2004	2011	rVB3	468524	672292	18.70%	1.703%
43	14.045	2028	2033	2036	rBV2	1288948	1453443	40.42%	3.683%
44	14.068	2036	2037	2041	rVB	358008	265427	7.38%	0.673%
45	14.198	2056	2059	2061	rBV	88508	89909	2.50%	0.228%
46	14.274	2068	2072	2075	rBV3	33514	49117	1.37%	0.124%
47	14.433	2097	2099	2102	rVB	76622	60240	1.68%	0.153%
48	14.468	2102	2105	2107	rBV	38734	41627	1.16%	0.105%
49	14.504	2108	2111	2118	rVB5	138719	220001	6.12%	0.557%
50	14.810	2161	2163	2167	rVB	95716	82974	2.31%	0.210%
51	15.098	2208	2212	2215	rBV	401113	580410	16.14%	1.471%
52	15.151	2219	2221	2224	rVV	112061	110950	3.09%	0.281%
53	15.410	2261	2265	2270	rVB	221053	291902	8.12%	0.740%
54	15.474	2271	2276	2280	rVB	294181	379679	10.56%	0.962%
55	15.539	2282	2287	2290	rBV	882915	1141087	31.73%	2.891%
56	15.980	2358	2362	2367	rBV	115910	168794	4.69%	0.428%
57	16.039	2367	2372	2381	rVV6	137546	286330	7.96%	0.725%
58	17.039	2536	2542	2548	rBV2	178507	331572	9.22%	0.840%
59	17.498	2615	2620	2629	rVB	122099	253825	7.06%	0.643%

Sum of corrected areas: 39466664

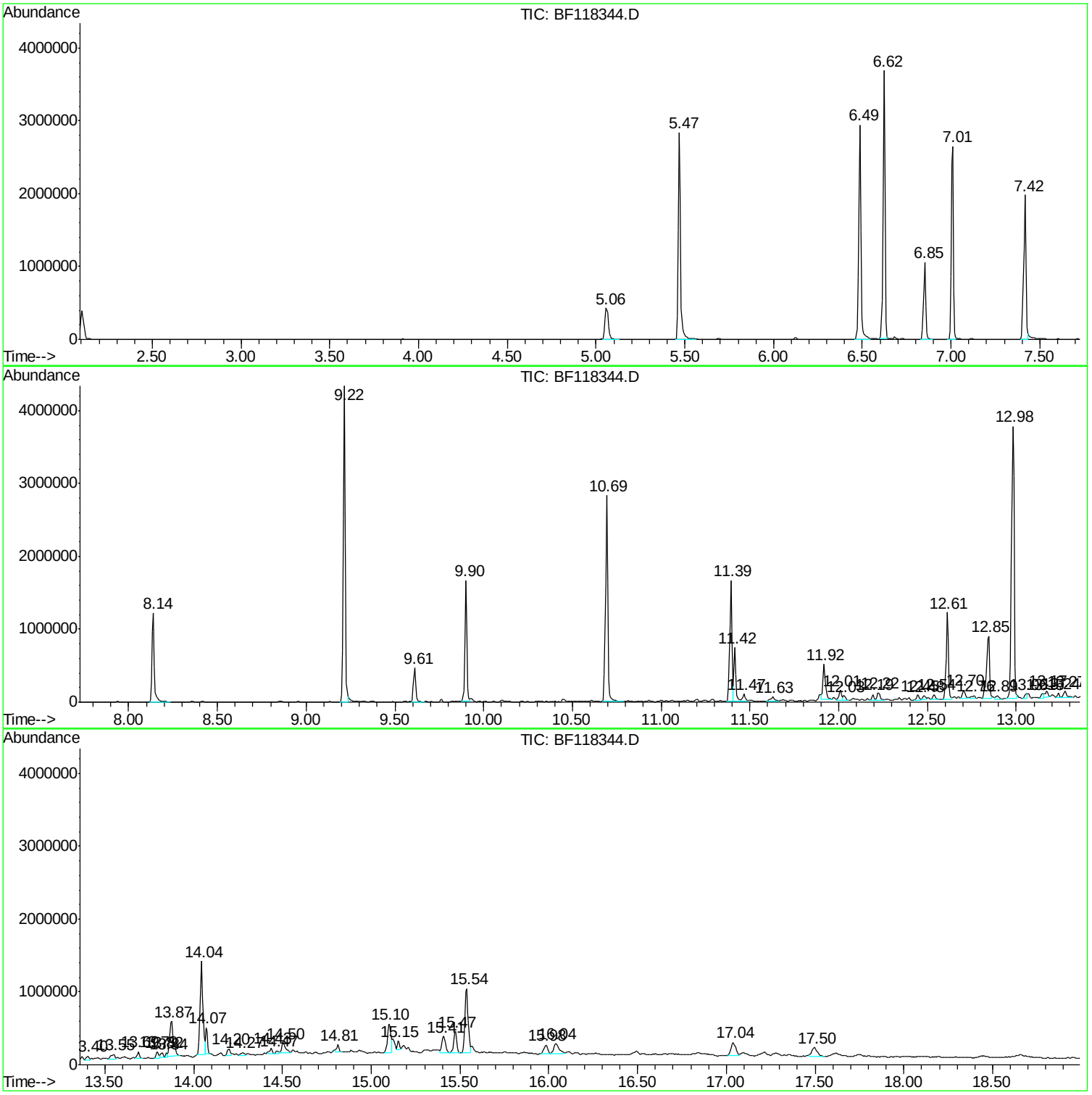
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118344.D
Acq On : 27 Dec 2019 18:11
Operator : JU
Sample : K6431-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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\BF122719\
Data File : BF118344.D
Acq On : 27 Dec 2019 18:11
Operator : JU
Sample : K6431-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4-(0-2)

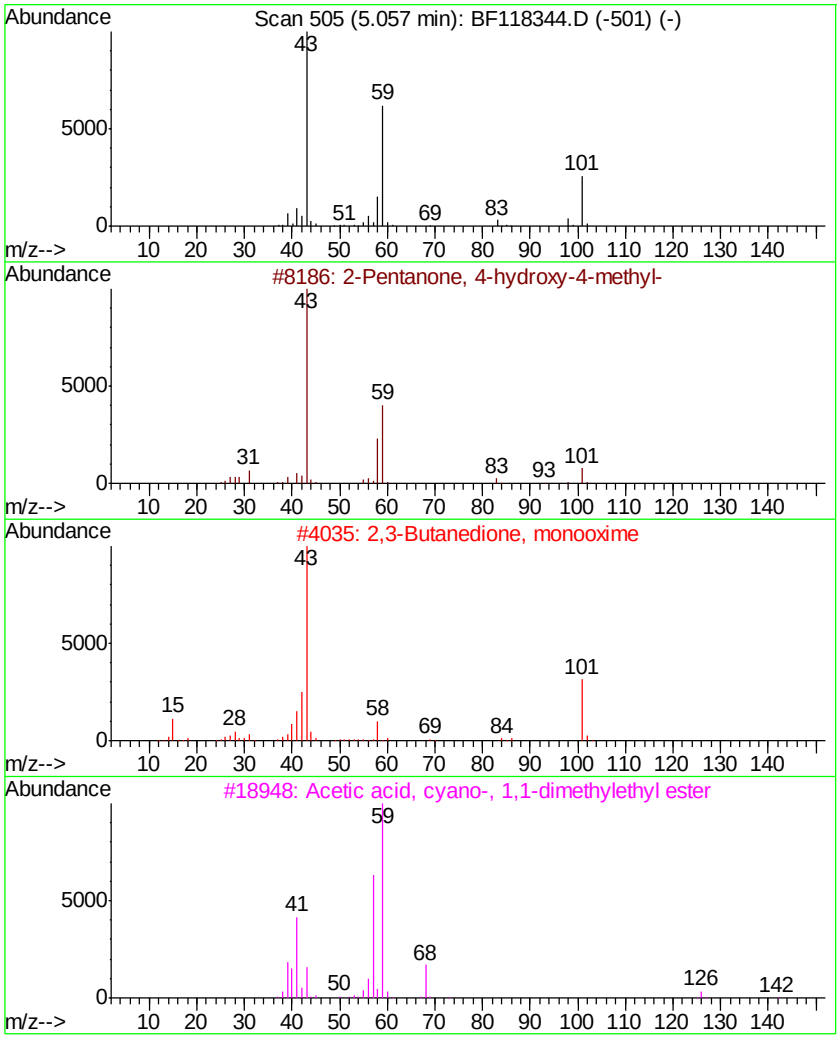
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

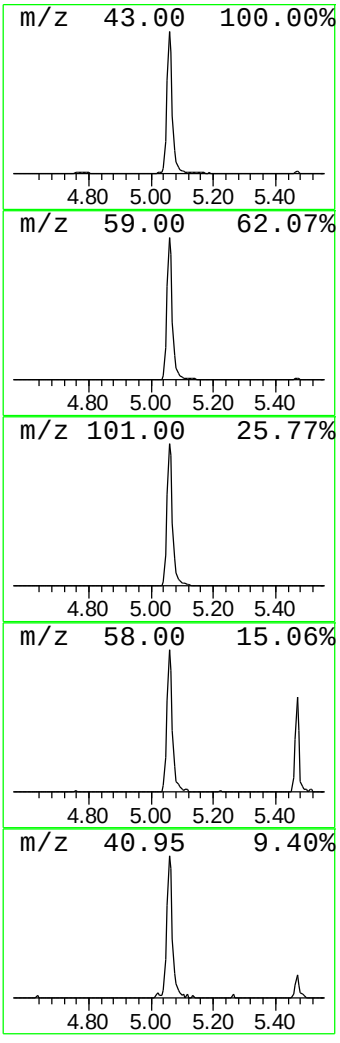
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	12.30 ng	535253	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
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Operator : JU
Sample : K6431-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

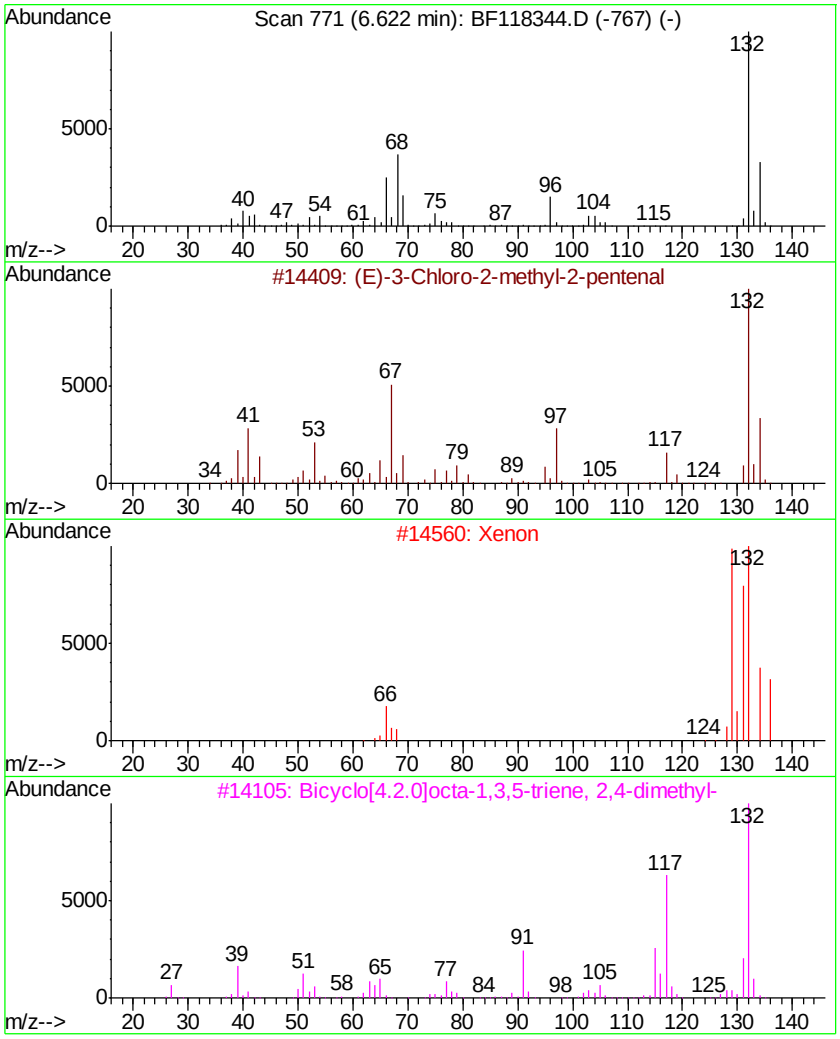
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

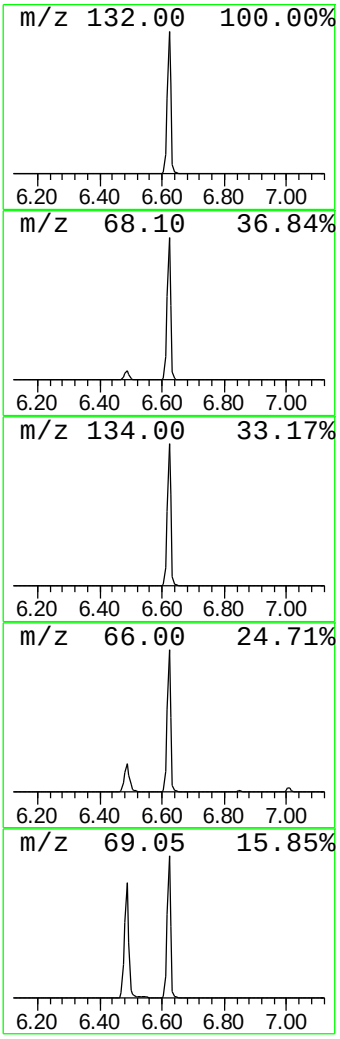
****

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	70.34 ng	3061080	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
2	Xenon	132	Xe	007440-63-3	9
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118344.D
Acq On : 27 Dec 2019 18:11
Operator : JU
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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

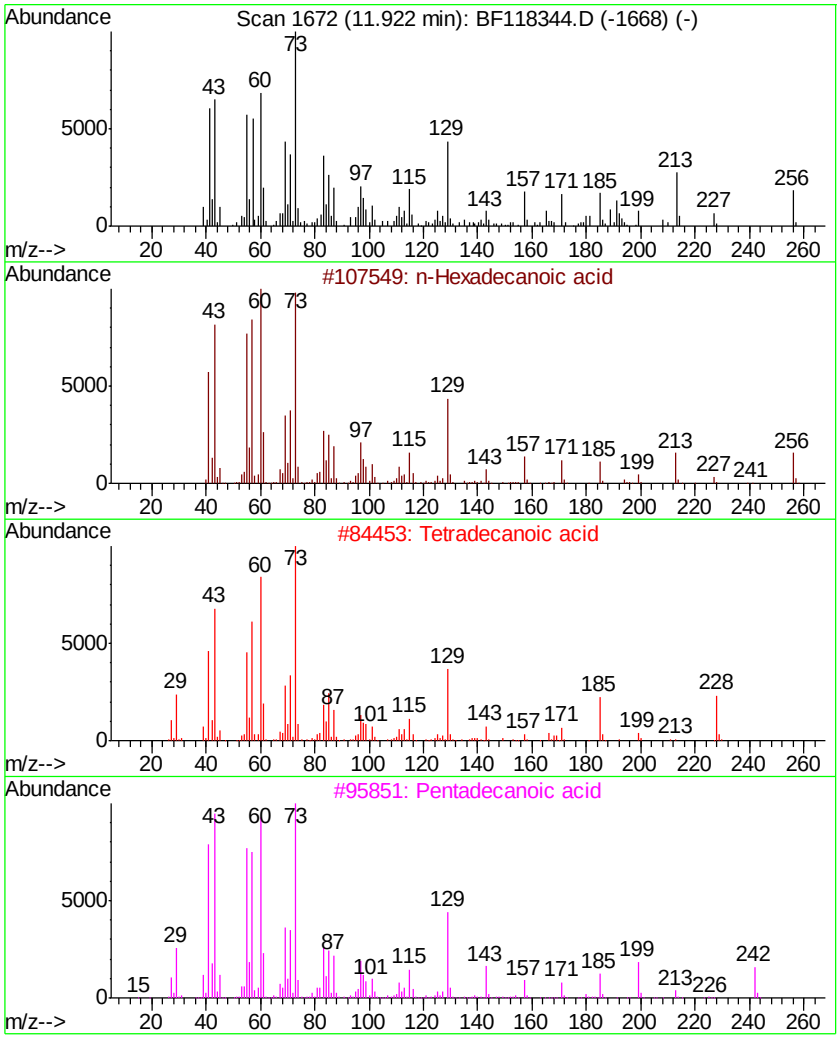
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

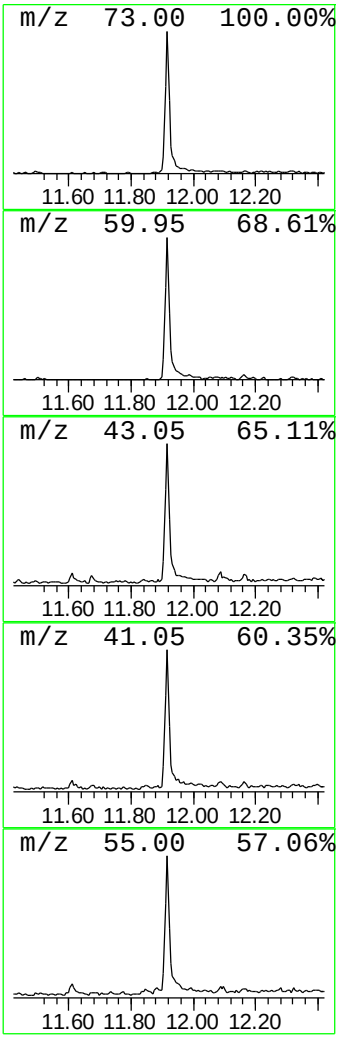
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	7.44 ng	514605	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	Dodecanoic acid	200	C12H24O2	000143-07-7	68





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118344.D
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Operator : JU
Sample : K6431-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

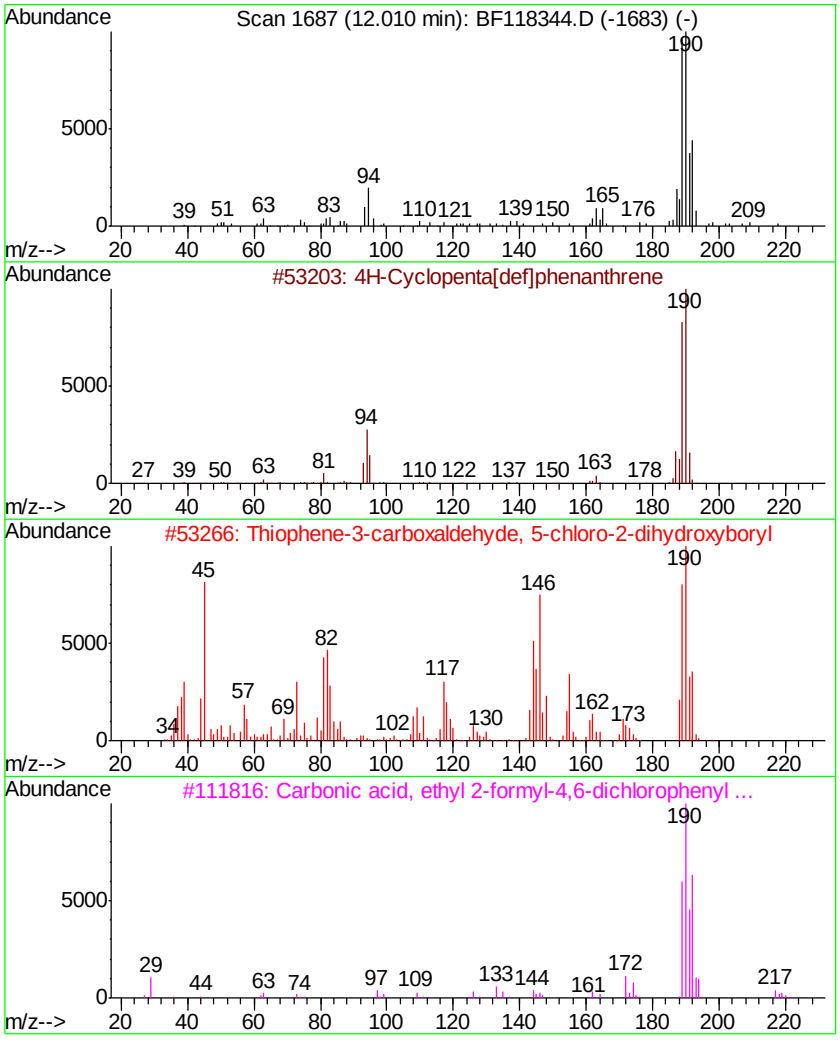
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

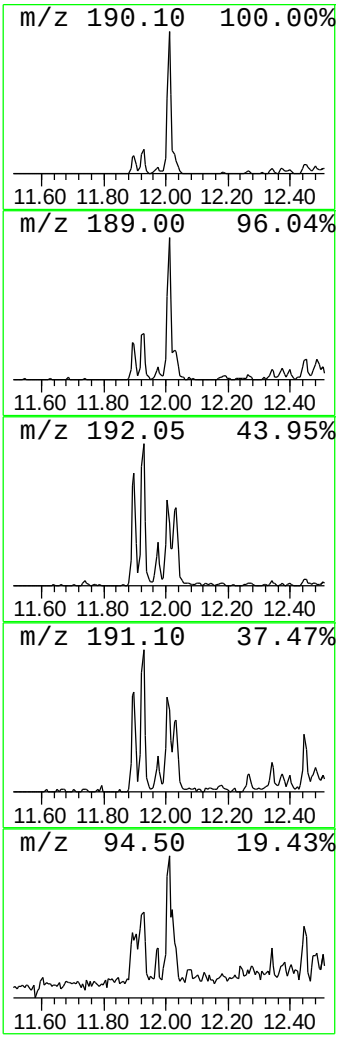
****

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	2.10 ng	145474	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	50
3	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	47
4	Methyl diselenide	190	C2H6Se2	007101-31-7	43
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	37





Library Search Compound Report

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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

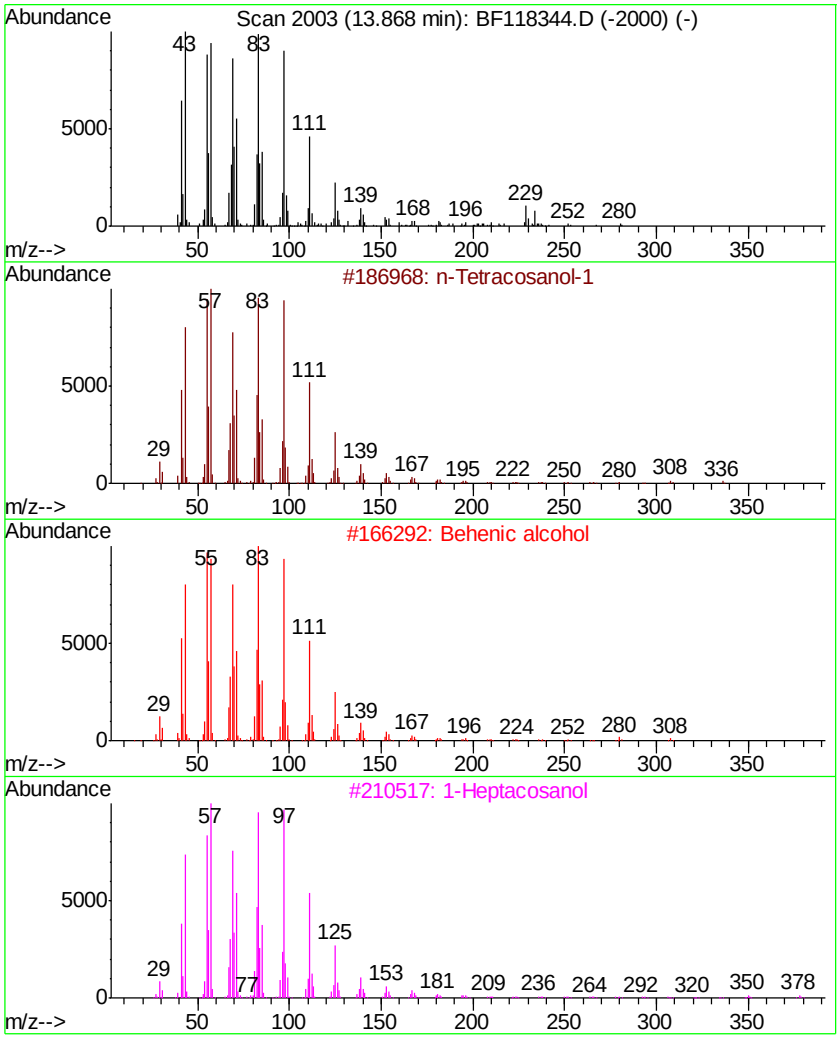
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

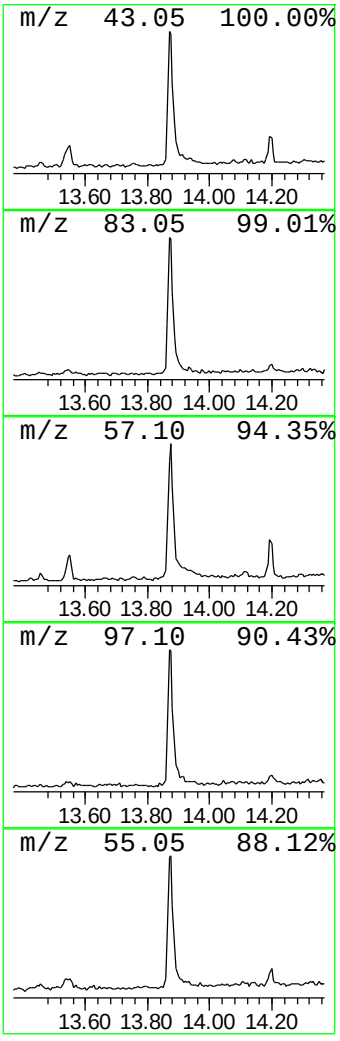
****

Peak Number 6 n-Tetracosanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	9.25 ng	672292	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
2	Behenic alcohol	326	C22H46O	000661-19-8	93
3	1-Heptacosanol	396	C27H56O	002004-39-9	93
4	9-Nonadecene	266	C19H38	031035-07-1	91
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	90





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Data File : BF118344.D
Acq On : 27 Dec 2019 18:11
Operator : JU
Sample : K6431-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

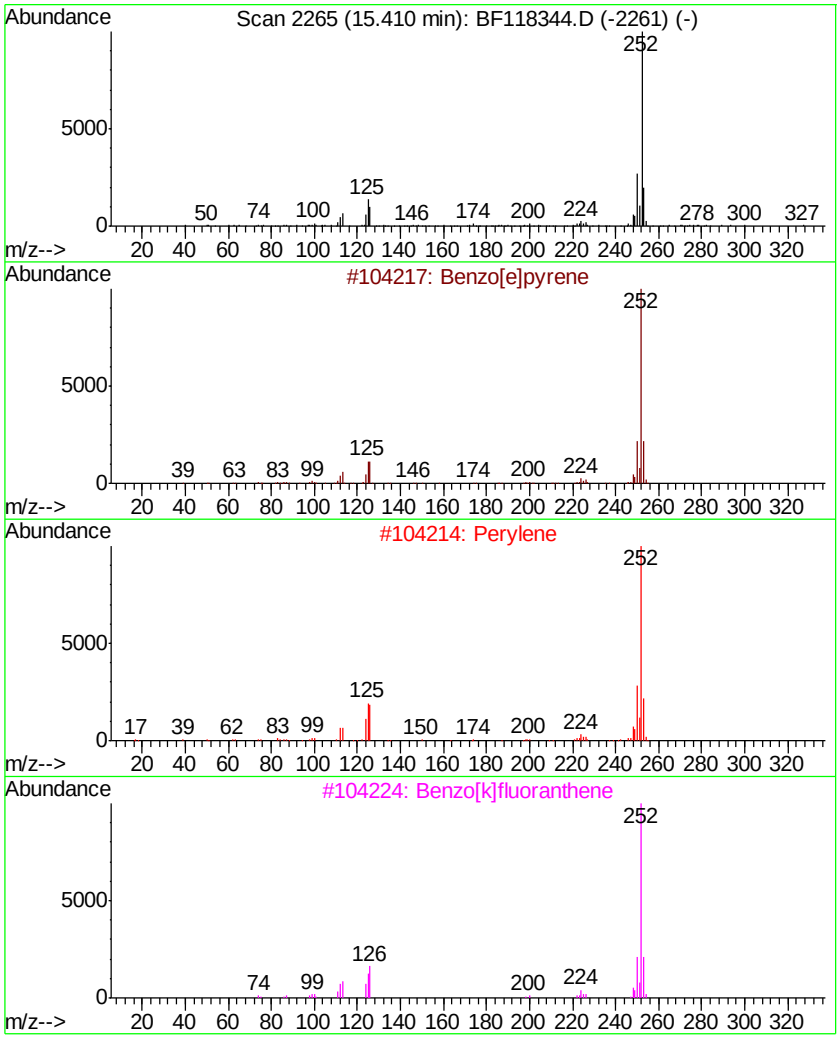
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

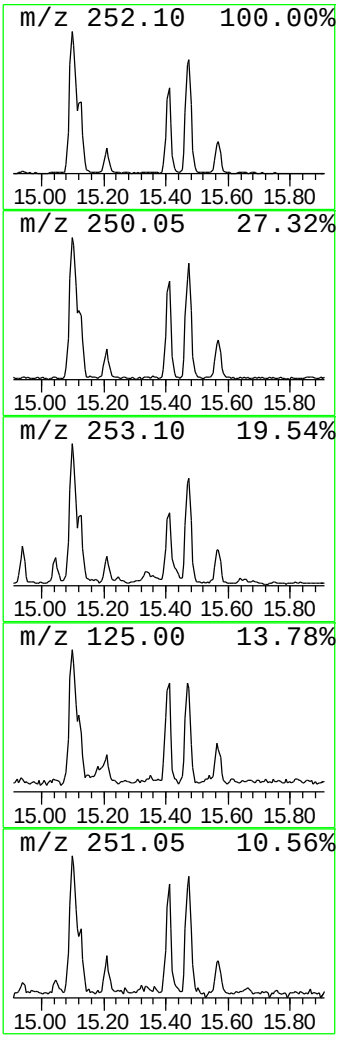
****

Peak Number 8 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.41	5.12 ng	291902	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Perylene	252	C20H12	000198-55-0	96
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
5	Benzo[a]pyrene	252	C20H12	000050-32-8	94





Library Search Compound Report

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Data File : BF118344.D
Acq On : 27 Dec 2019 18:11
Operator : JU
Sample : K6431-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

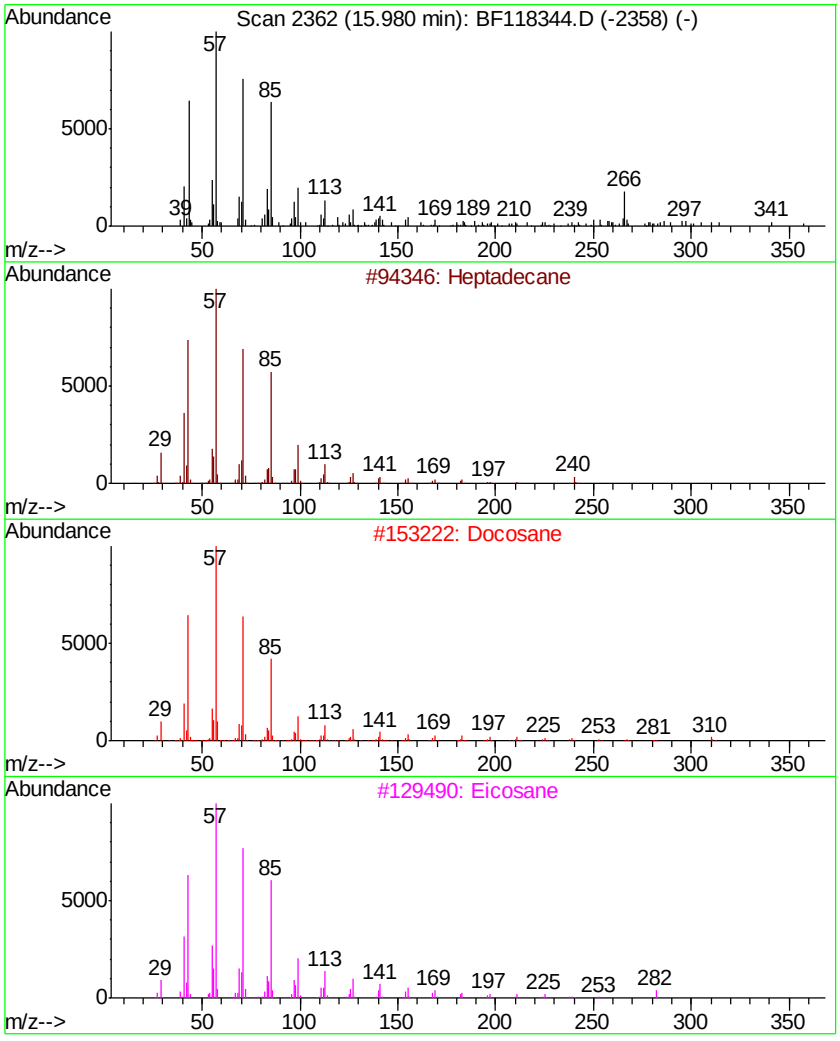
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

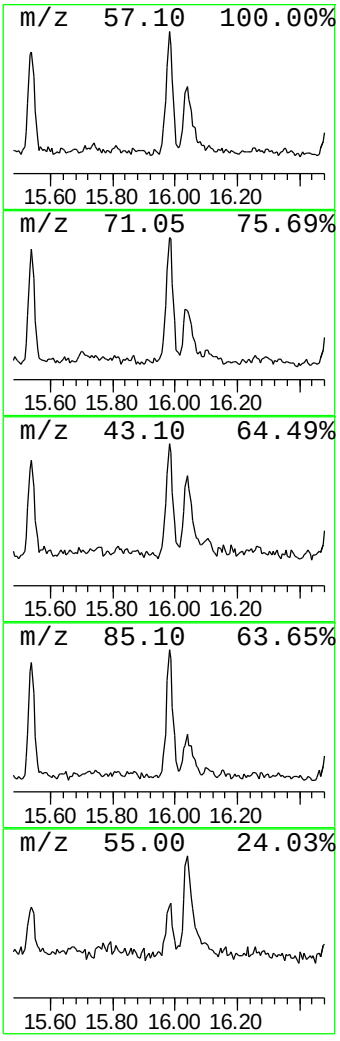
****

Peak Number 9 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.98	2.96 ng	168794	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Docosane	310	C22H46	000629-97-0	90
3	Eicosane	282	C20H42	000112-95-8	87
4	Heneicosane	296	C21H44	000629-94-7	87
5	Tetracosane	338	C24H50	000646-31-1	83





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118344.D
Acq On : 27 Dec 2019 18:11
Operator : JU
Sample : K6431-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

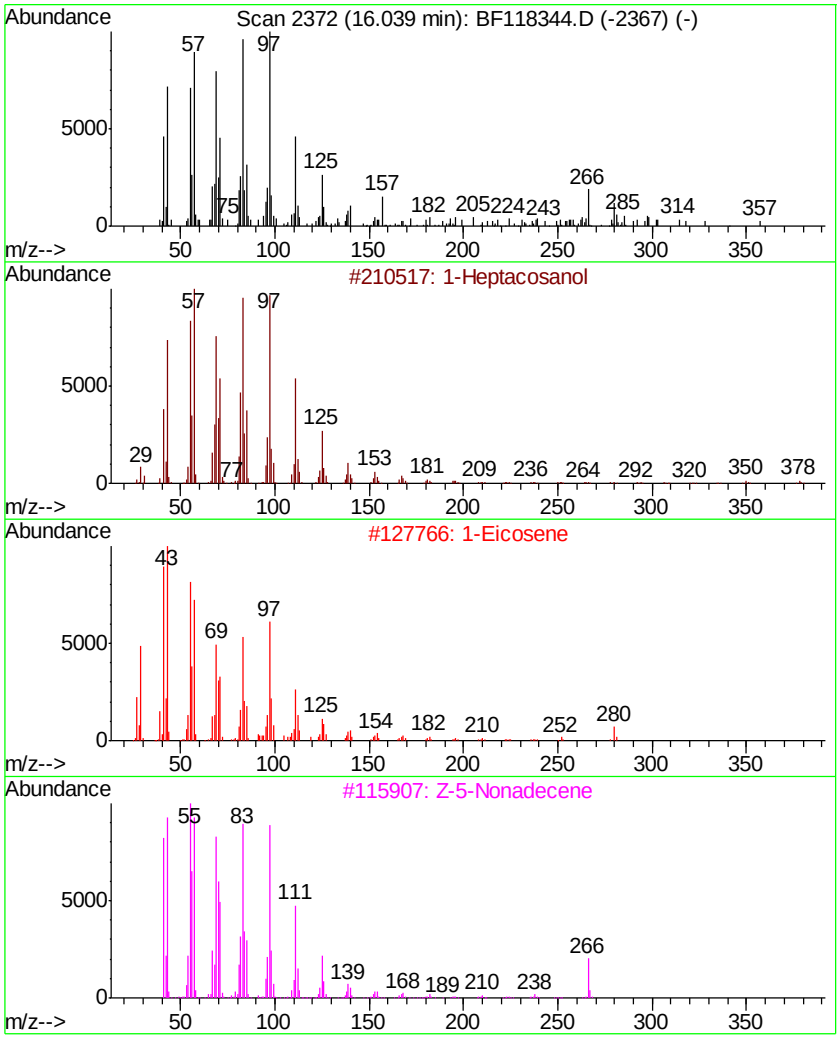
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

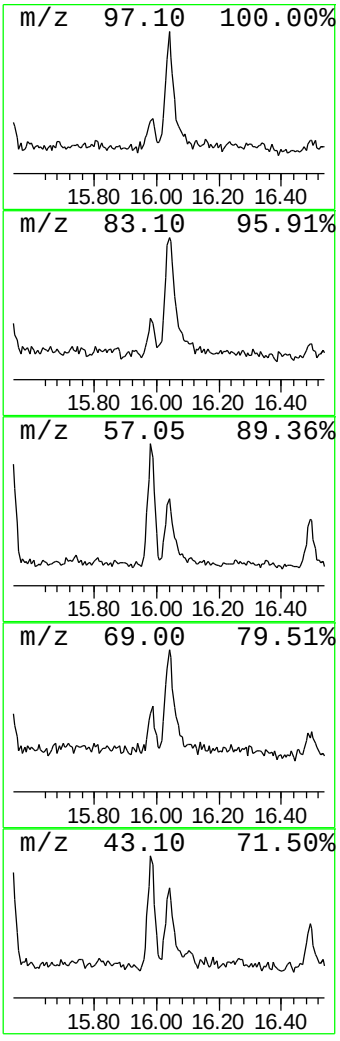
****

Peak Number 10 1-Heptacosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.04	5.02 ng	286330	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	91
2	1-Eicosene	280	C20H40	003452-07-1	89
3	Z-5-Nonadecene	266	C19H38	1000131-11-8	89
4	8-Heptadecene	238	C17H34	002579-04-6	87
5	1-Nonadecene	266	C19H38	018435-45-5	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF122719\
Data File : BF118344.D
Acq On : 27 Dec 2019 18:11
Operator : JU
Sample : K6431-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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	12.3	ng	535253	1	6.85	870339	20.0
unknown6.62	6.62	70.3	ng	3061080	1	6.85	870339	20.0
n-Hexadecanoic acid	11.92	7.4	ng	514605	4	11.39	1383040	20.0
4H-Cyclopenta[def...	12.01	2.1	ng	145474	4	11.39	1383040	20.0
n-Tetracosanol-1	13.87	9.3	ng	672292	5	14.04	1453440	20.0
Benzo[e]pyrene	15.41	5.1	ng	291902	6	15.54	1141090	20.0
Heptadecane	15.98	3.0	ng	168794	6	15.54	1141090	20.0
1-Heptacosanol	16.04	5.0	ng	286330	6	15.54	1141090	20.0