LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071719\
Data File : BF115636.D
Acq On : 17 Jul 2019 21:39
Operator : HP/JU
Sample : K3835-31 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-7(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-BF071219.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	2.187	12	17	28	rVB	355224	453153	24.24%	1.924%
2	5.098	504	512	520	rBV2	21041	32193	1.72%	0.137%
3	5.498	576	580	598	rVB	1457345	1460974	78.15%	6.203%
4	6.504	747	751	758	rBV	1768774	1563054	83.61%	6.637%
5	6.563	758	761	764	rVB2	30009	30949	1.66%	0.131%
6	6.651	772	776	779	rBV	2015435	1677999	89.76%	7.125%
7	6.881	811	815	819	rBV	1368362	1106971	59.22%	4.700%
8	7.039	838	842	845	rBV	1594358	1332196	71.26%	5.657%
9	7.257	876	879	886	rBV2	16588	25491	1.36%	0.108%
10	7.433	905	909	915	rBV	1056974	963434	51.54%	4.091%
11	8.163	1029	1033	1036	rBV	1698356	1390325	74.37%	5.903%
12	8.216	1040	1042	1049	rVB2	16594	23471	1.26%	0.100%
13	9.233	1211	1215	1218	rBV	2367540	1869384	100.00%	7.938%
14	9.598	1275	1277	1278	rBV	55619	38388	2.05%	0.163%
15	9.622	1278	1281	1287	rVB	550995	427293	22.86%	1.814%
16	9.757	1301	1304	1310	rBV2	59230	70835	3.79%	0.301%
17	9.916	1327	1331	1335	rBV	1476700	1287824	68.89%	5.468%
18	10.286	1391	1394	1397	rVB	52025	39583	2.12%	0.168%
19	10.427	1415	1418	1421	rBV	57736	46250	2.47%	0.196%
20	10.698	1460	1464	1474	rBV	872698	768833	41.13%	3.265%
21	10.822	1482	1485	1493	rVB4	19845	30041	1.61%	0.128%
22	11.398	1579	1583	1585	rBV	1193681	1048724	56.10%	4.453%
23	11.416	1585	1586	1590	rVV	173993	133438	7.14%	0.567%
24	11.451	1590	1592	1594	rVV	57113	49250	2.63%	0.209%
25	11.469	1594	1595	1598	rVB	45738	27911	1.49%	0.119%
26	11.621	1616	1621	1623	rBV2	20602	25177	1.35%	0.107%
27	11.898	1662	1668	1669	rBV	30357	33928	1.81%	0.144%
28	11.921	1669	1672	1679	rVV3	221442	236452	12.65%	1.004%
29	12.010	1683	1687	1689	rBV2	36953	39101	2.09%	0.166%
30	12.098	1699	1702	1704	rBV	25576	24830	1.33%	0.105%
31	12.192	1712	1718	1719	rBV2	29374	29513	1.58%	0.125%
32	12.210	1719	1721	1726	rVB2	34043	33546	1.79%	0.142%
33	12.445	1759	1761	1764	rBV	32935	30699	1.64%	0.130%
34	12.486	1764	1768	1772	rVB2	33910	40851	2.19%	0.173%

LSC Area Percent Report

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Acq On : 17 Jul 2019 21:39
Operator : HP/JU
Sample : K3835-31 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-7(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-BF071219.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.527	1772	1775	1780	rVB2	34811	38044	2.04%	0.162%
36	12.580	1781	1784	1786	rBV2	45864	46513	2.49%	0.197%
37	12.604	1786	1788	1792	rVB	346491	295620	15.81%	1.255%
38	12.704	1801	1805	1807	rBV	70711	69570	3.72%	0.295%
39	12.833	1821	1827	1830	rBV	337619	364674	19.51%	1.548%
40	12.880	1833	1835	1840	rVB3	22453	25821	1.38%	0.110%
41	12.974	1847	1851	1859	rVB	1425604	1208851	64.67%	5.133%
42	13.057	1860	1865	1867	rBV2	25774	41134	2.20%	0.175%
43	13.163	1880	1883	1885	rVB2	54683	51150	2.74%	0.217%
44	13.210	1888	1891	1892	rVV	33259	27206	1.46%	0.116%
45	13.227	1892	1894	1896	rVV	49900	41489	2.22%	0.176%
46	13.263	1897	1900	1904	rVB2	35904	43492	2.33%	0.185%
47	13.386	1919	1921	1925	rBV4	28057	36919	1.97%	0.157%
48	13.668	1966	1969	1974	rVB	60384	63724	3.41%	0.271%
49	13.780	1983	1988	1989	rBV2	65061	88406	4.73%	0.375%
50	13.810	1991	1993	1994	rVV2	62272	51853	2.77%	0.220%
51	13.833	1994	1997	2001	rVB4	86046	118996	6.37%	0.505%
52	13.874	2002	2004	2005	rBV	41235	36676	1.96%	0.156%
53	14.027	2025	2030	2033	rBV2	999392	1171654	62.68%	4.975%
54	14.051	2033	2034	2042	rVB	208049	194468	10.40%	0.826%
55	14.192	2056	2058	2060	rBV	37415	29506	1.58%	0.125%
56	14.498	2108	2110	2113	rVV2	85833	66902	3.58%	0.284%
57	14.539	2113	2117	2124	rVB7	110403	204200	10.92%	0.867%
58	14.804	2160	2162	2166	rVB	57842	50608	2.71%	0.215%
59	14.951	2183	2187	2189	rBV2	133913	158340	8.47%	0.672%
60	15.068	2203	2207	2210	rBV	203577	292599	15.65%	1.242%
61	15.145	2216	2220	2223	rBV	164800	193394	10.35%	0.821%
62	15.209	2227	2231	2246	rVB8	133892	442731	23.68%	1.880%
63	15.368	2255	2258	2262	rBV	134019	142133	7.60%	0.604%
64	15.433	2265	2269	2274	rVB	147950	186225	9.96%	0.791%
65	15.498	2275	2280	2283	rBV	683226	844897	45.20%	3.587%
66	15.727	2315	2319	2323	rVB2	197597	271166	14.51%	1.151%
67	15.962	2355	2359	2365	rVB	185398	260198	13.92%	1.105%

Sum of corrected areas: 23551220

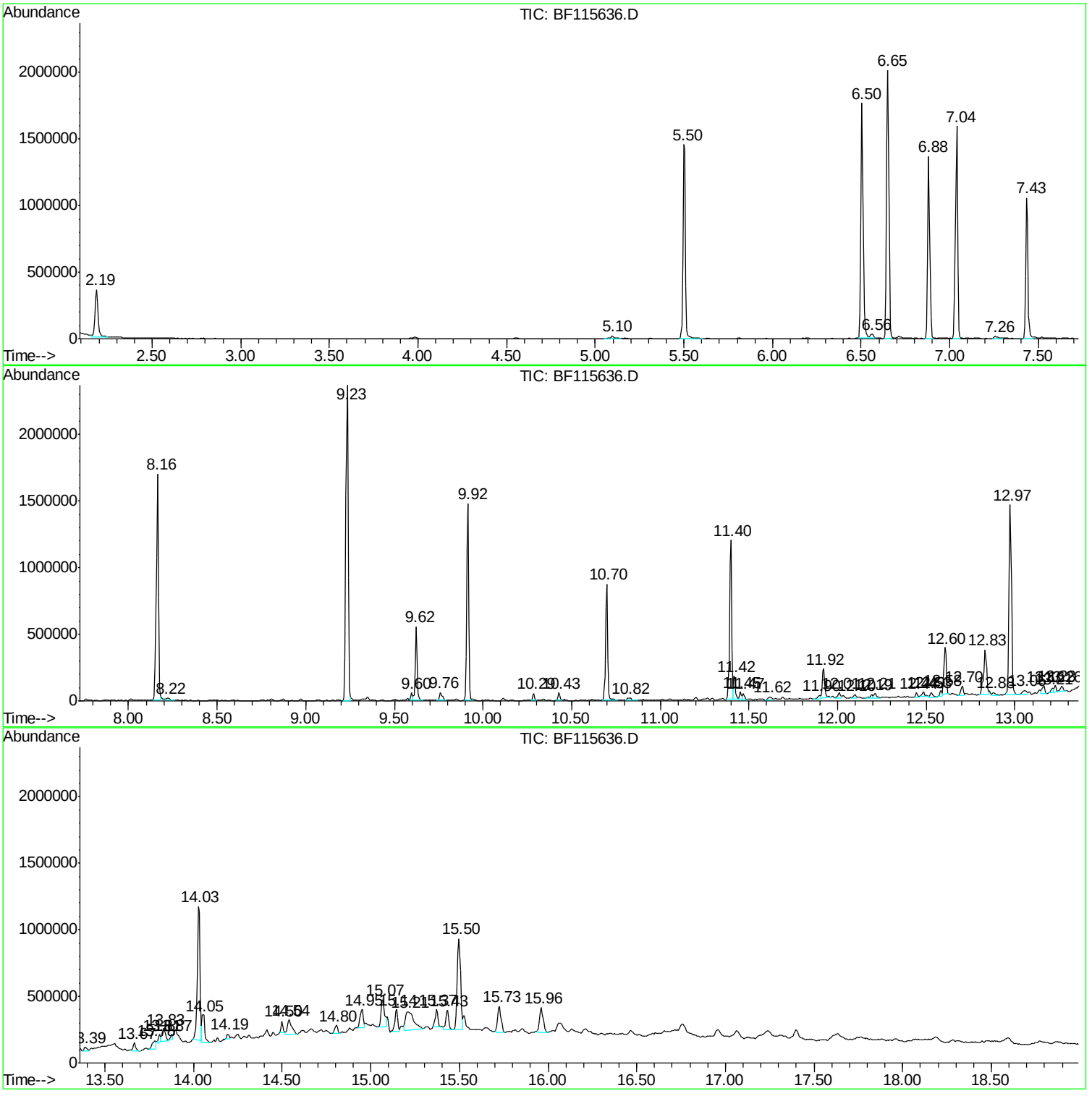
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071719\
Data File : BF115636.D
Acq On : 17 Jul 2019 21:39
Operator : HP/JU
Sample : K3835-31 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-7(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.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\BF071719\
Data File : BF115636.D
Acq On : 17 Jul 2019 21:39
Operator : HP/JU
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Misc :
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Instrument : BNA_F
ClientSampleId : SB-7(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

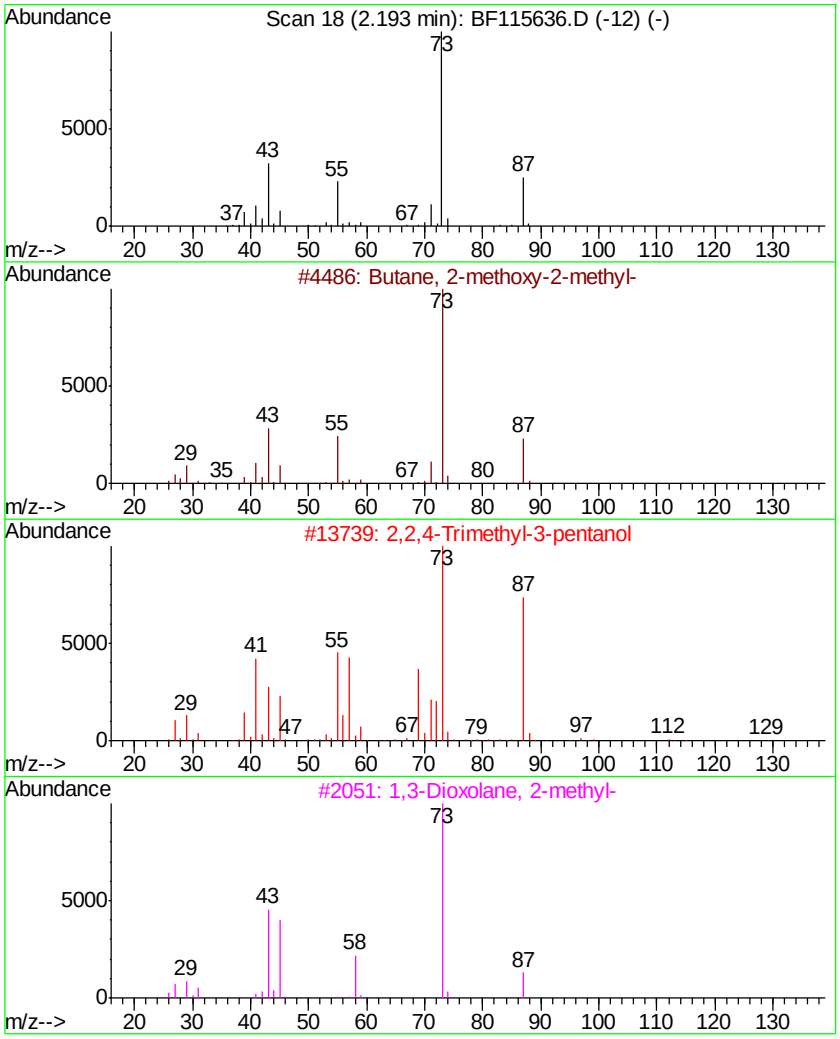
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

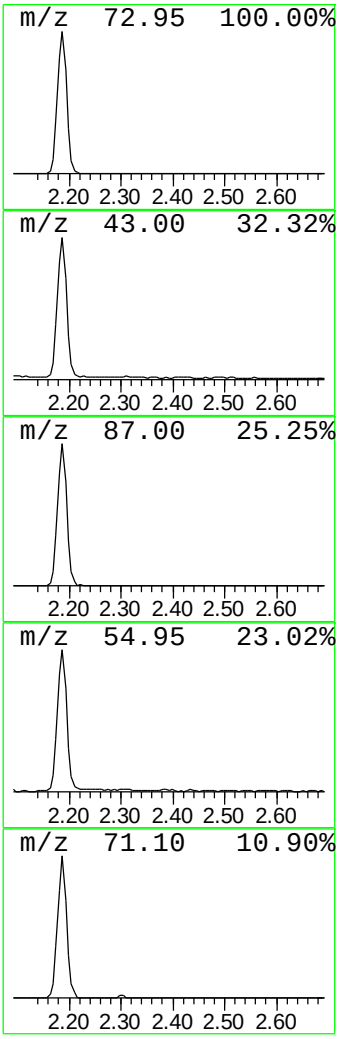
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.19	8.19 ng	453153	1,4-Dichlorobenzene-d4	6.88

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	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071719\
Data File : BF115636.D
Acq On : 17 Jul 2019 21:39
Operator : HP/JU
Sample : K3835-31 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-7(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

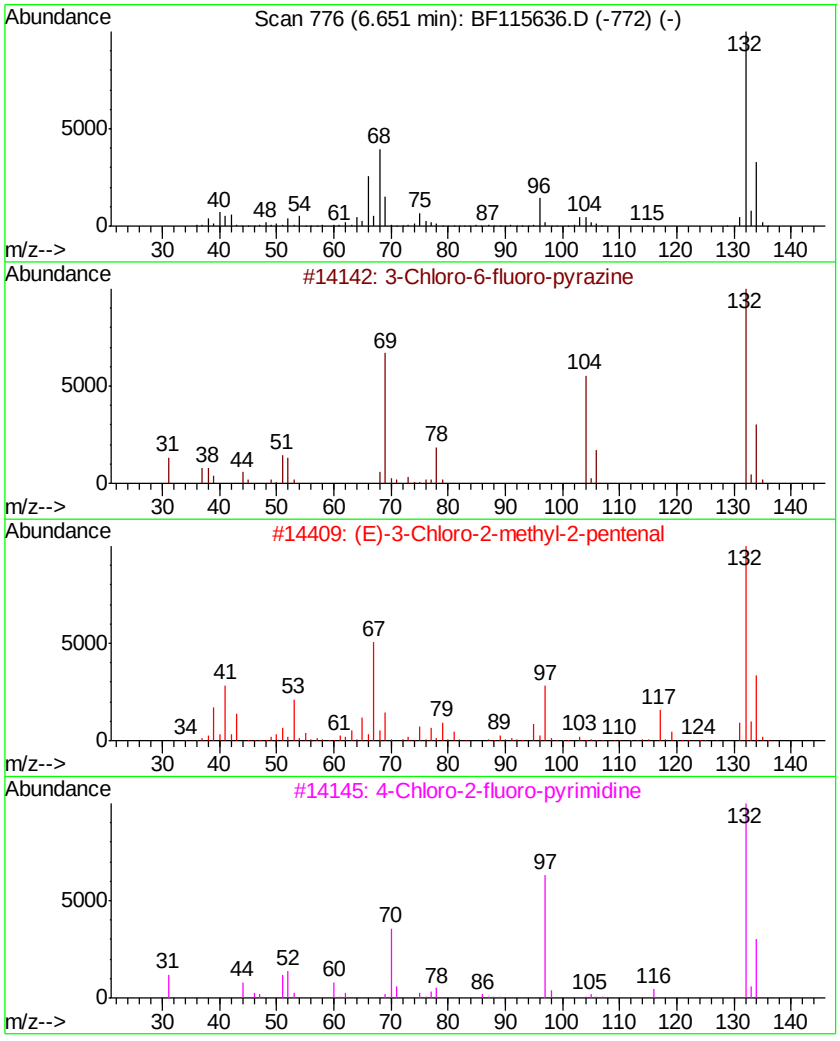
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

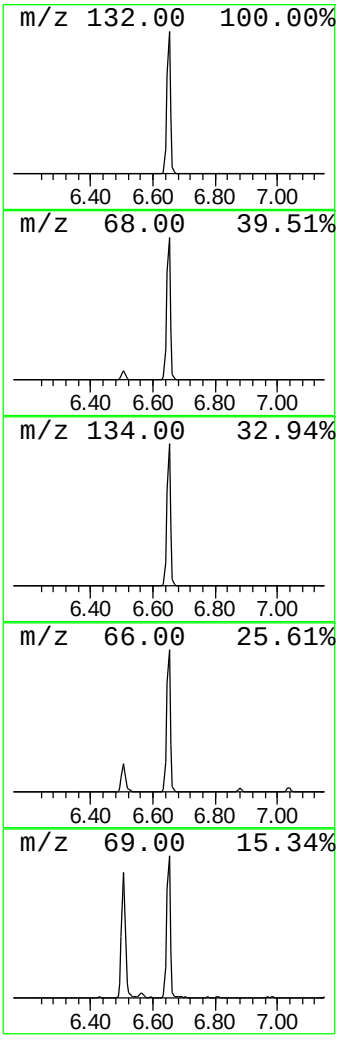
****

Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	30.32 ng	1678000	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	Xenon	132	Xe	007440-63-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071719\
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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-7(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

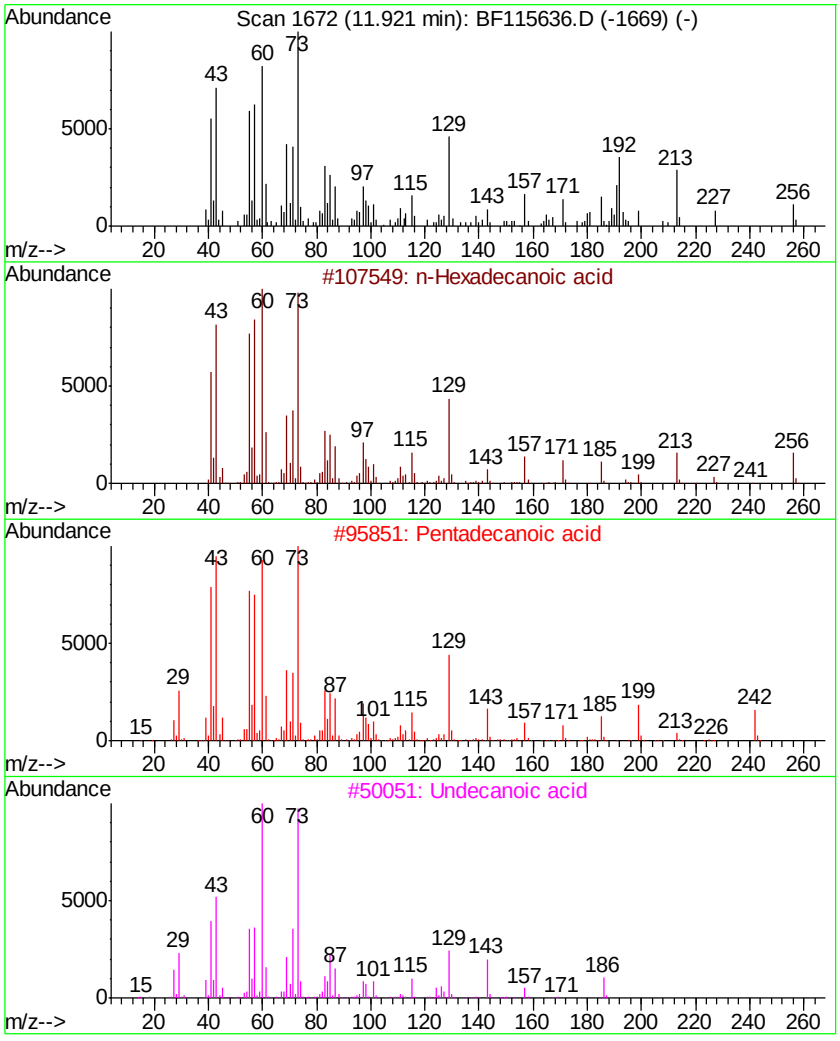
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

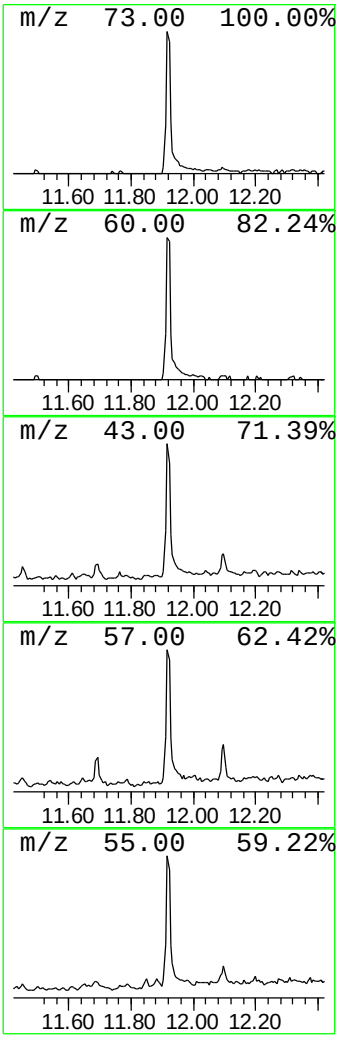
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	4.51 ng	236452	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3	Undecanoic acid	186	C11H22O2	000112-37-8	68
4	Tridecanoic acid	214	C13H26O2	000638-53-9	68
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071719\
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Sample : K3835-31 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-7(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

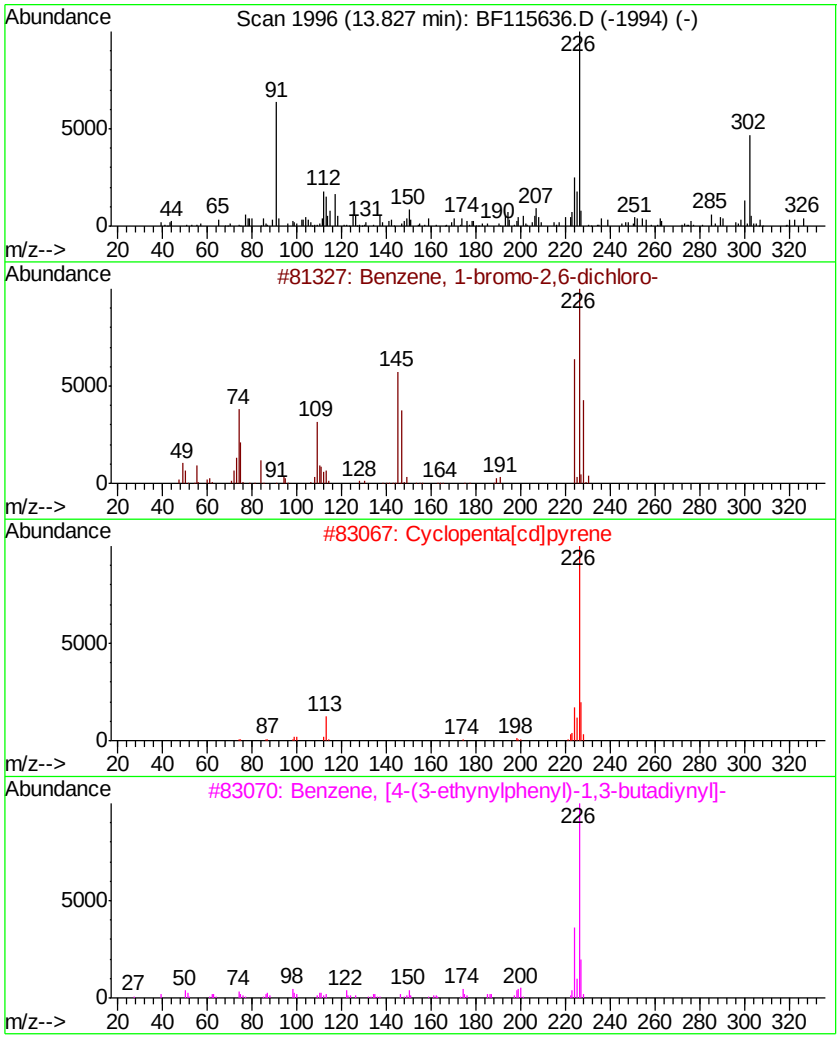
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

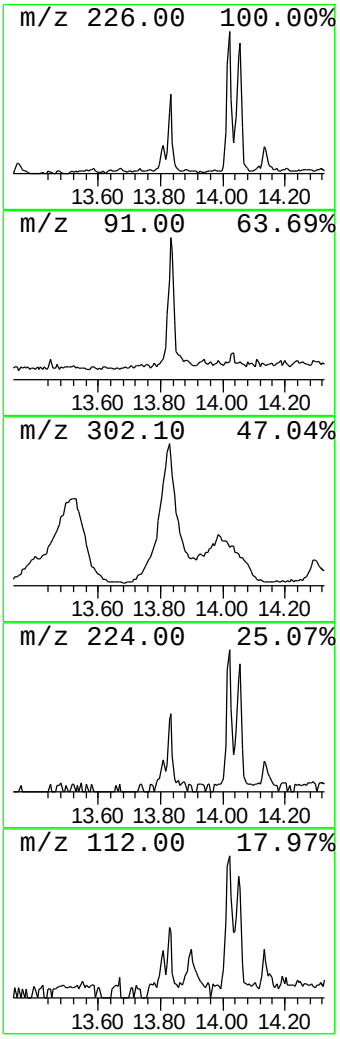
****

Peak Number 5 unknown13.83 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	2.03 ng	118996	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-bromo-2,6-dichloro-	224	C6H3BrCl2	019393-92-1	46
2	Cyclopenta[cd]pyrene	226	C18H10	027208-37-3	46
3	Benzene, [4-(3-ethynylphenyl)-1,...	226	C18H10	1000115-87-3	37
4	6-Methyl-4-phenyl-3-cyanopyridin...	226	C13H10N2S	078564-23-5	32
5	Imidazole, 5-methyl-4-trifluorom...	226	C11H9F3N2	081769-66-6	32





Library Search Compound Report

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Acq On : 17 Jul 2019 21:39
Operator : HP/JU
Sample : K3835-31 2X
Misc :
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Instrument : BNA_F
ClientSampleId : SB-7(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

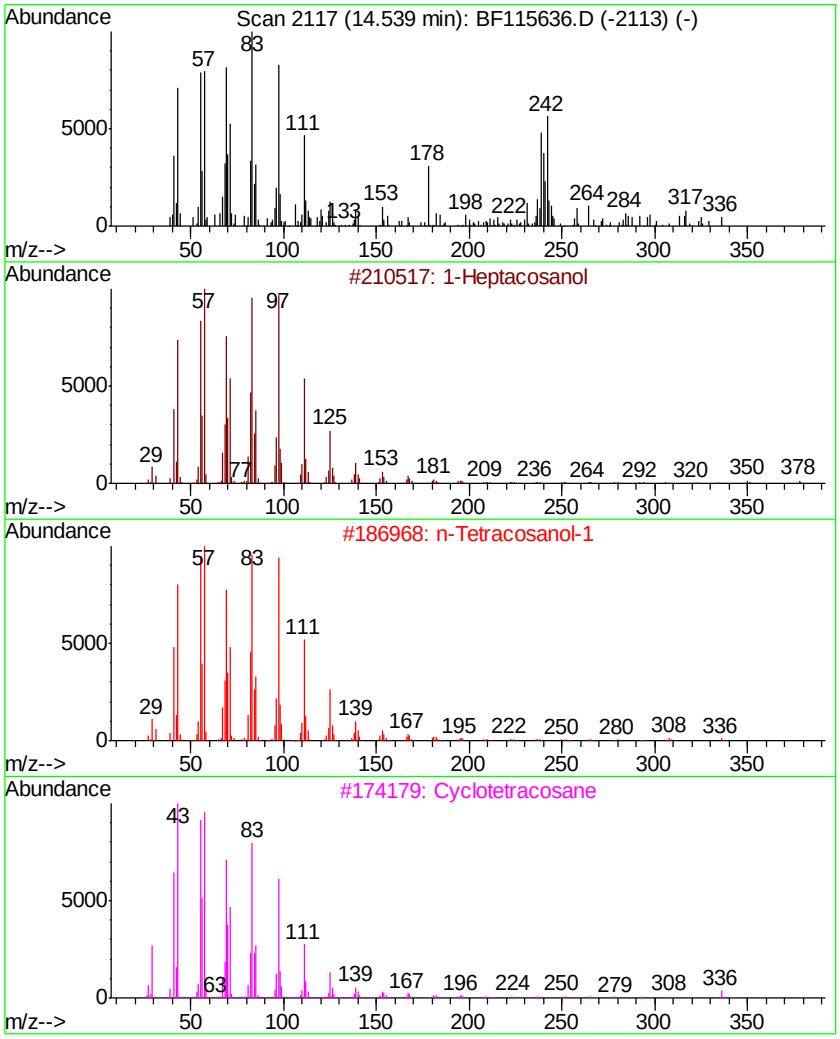
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

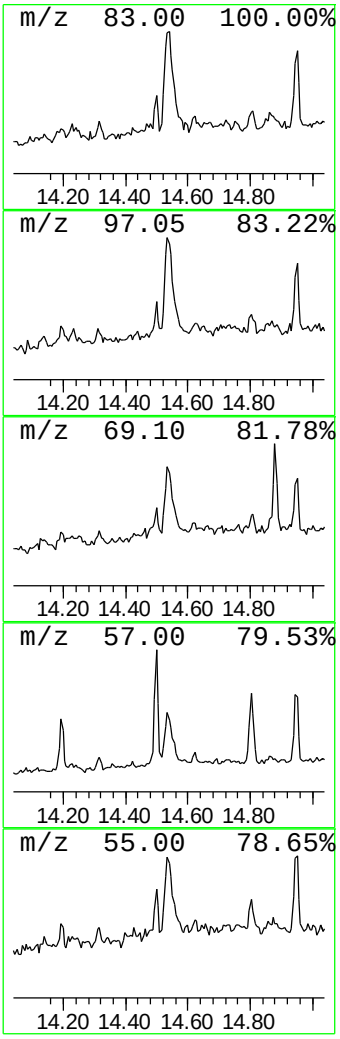
****

Peak Number 6 1-Heptacosanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.54	3.49 ng	204200	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	83
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	64
3	Cyclotetracosane	336	C24H48	000297-03-0	55
4	1-Docosene	308	C22H44	001599-67-3	52
5	Behenic alcohol	326	C22H46O	000661-19-8	52





Library Search Compound Report

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Sample : K3835-31 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-7(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

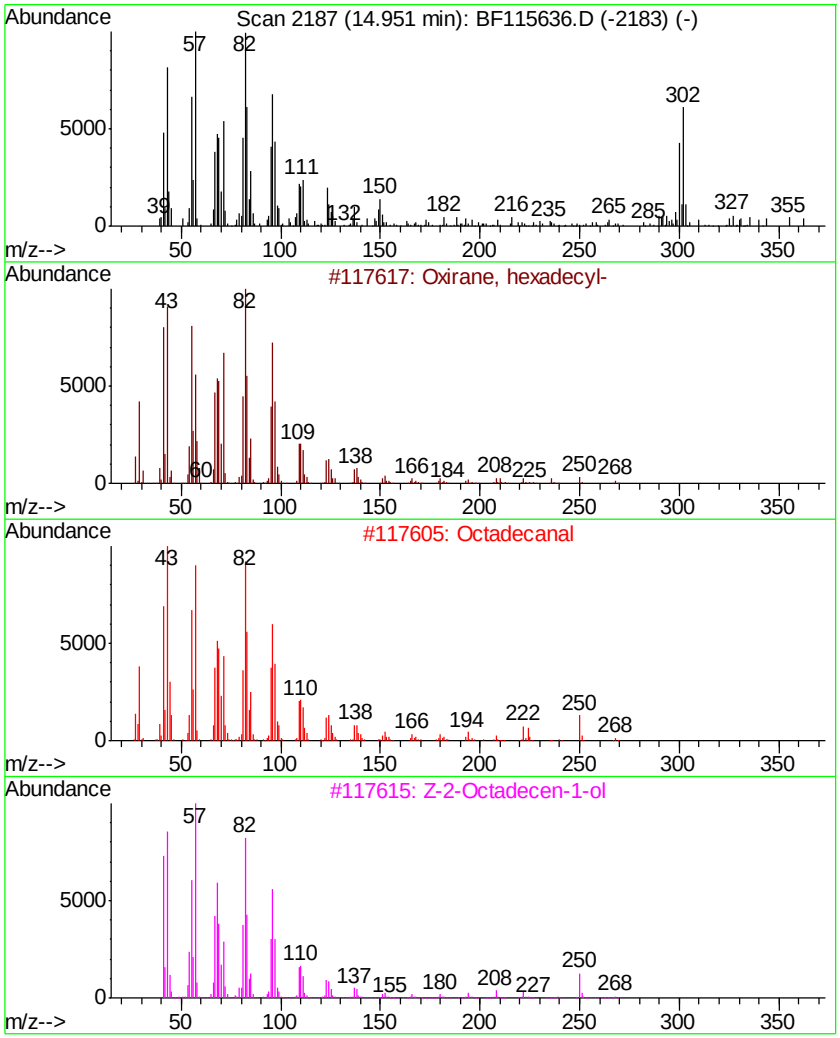
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

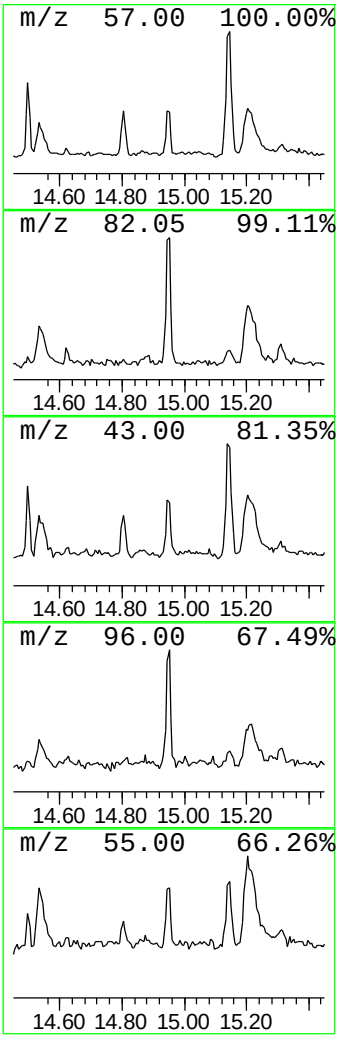
****

Peak Number 7 Oxirane, hexadecyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	3.75 ng	158340	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	93
2	Octadecanal	268	C18H36O	000638-66-4	92
3	Z-2-Octadecen-1-ol	268	C18H36O	1000131-11-0	78
4	18-Nonadecen-1-ol	282	C19H38O	1000142-89-2	58
5	16-Heptadecenal	252	C17H32O	1000144-57-9	53





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071719\
Data File : BF115636.D
Acq On : 17 Jul 2019 21:39
Operator : HP/JU
Sample : K3835-31 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-7(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

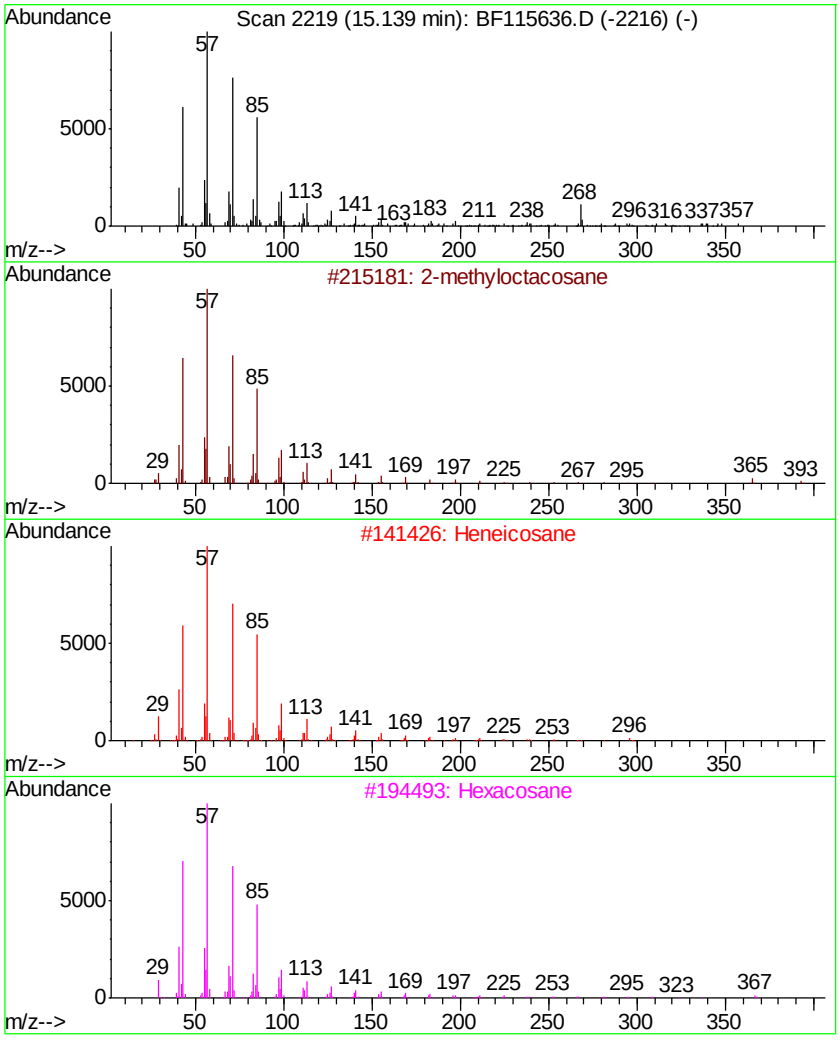
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

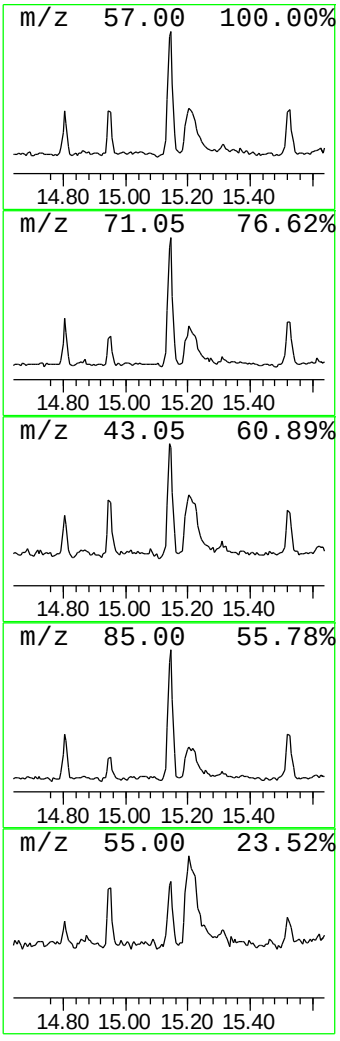
****

Peak Number 8 2-methyloctacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.14	4.58 ng	193394	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	90
2	Heneicosane	296	C21H44	000629-94-7	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
5	Heptadecane	240	C17H36	000629-78-7	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071719\
Data File : BF115636.D
Acq On : 17 Jul 2019 21:39
Operator : HP/JU
Sample : K3835-31 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-7(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

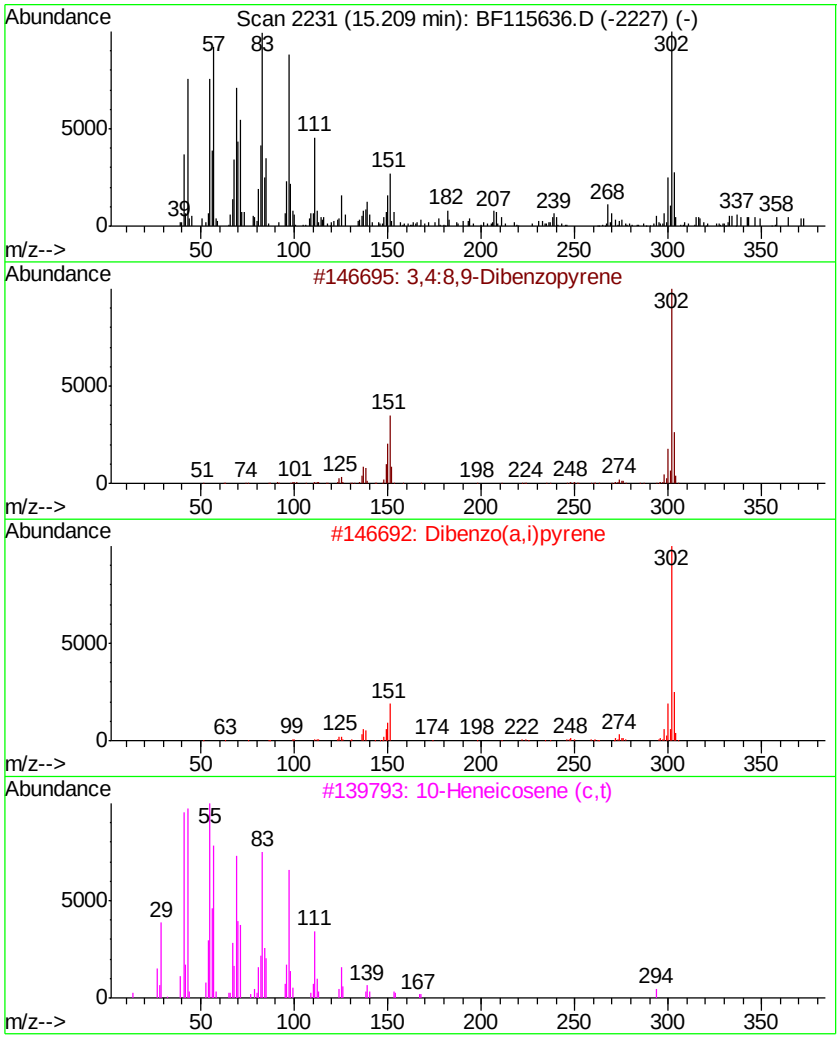
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

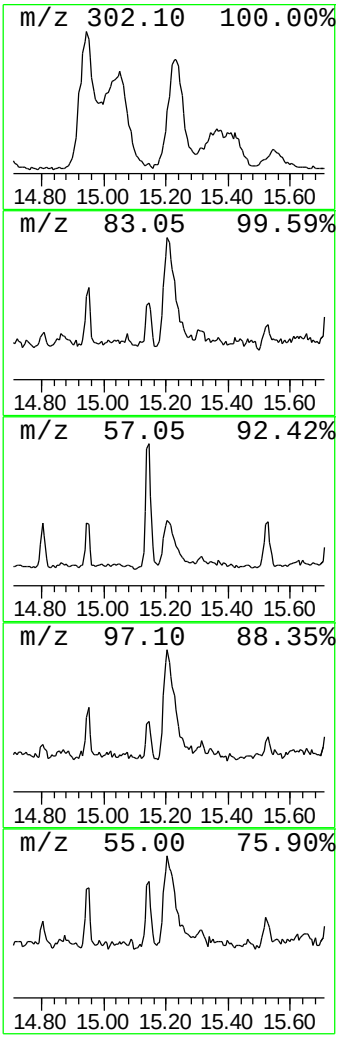
****

Peak Number 9 3,4:8,9-Dibenzopyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.21	10.48 ng	442731	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4:8,9-Dibenzopyrene	302	C24H14	000189-64-0	84
2	Dibenzo(a,i)pyrene	302	C24H14	000189-55-9	83
3	10-Heneicosene (c,t)	294	C21H42	095008-11-0	70
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	55
5	E-14-Hexadecenal	238	C16H30O	330207-53-9	55





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071719\
Data File : BF115636.D
Acq On : 17 Jul 2019 21:39
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Misc :
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Instrument : BNA_F
ClientSampleId : SB-7(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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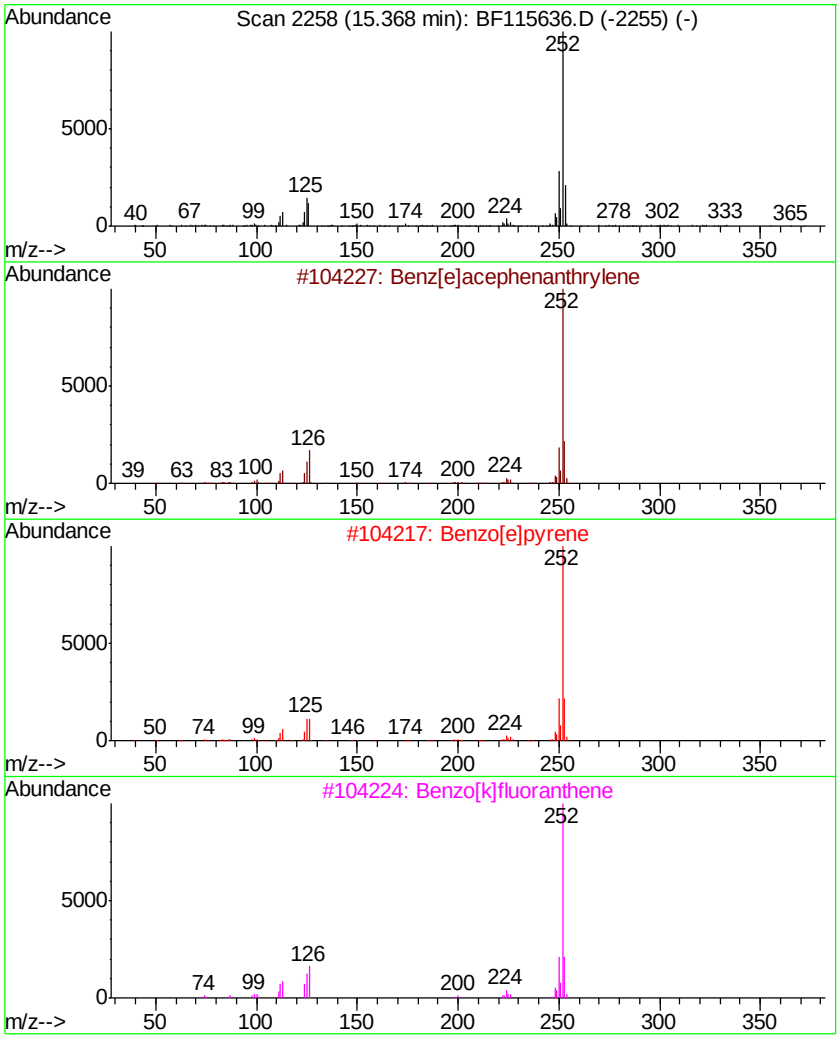
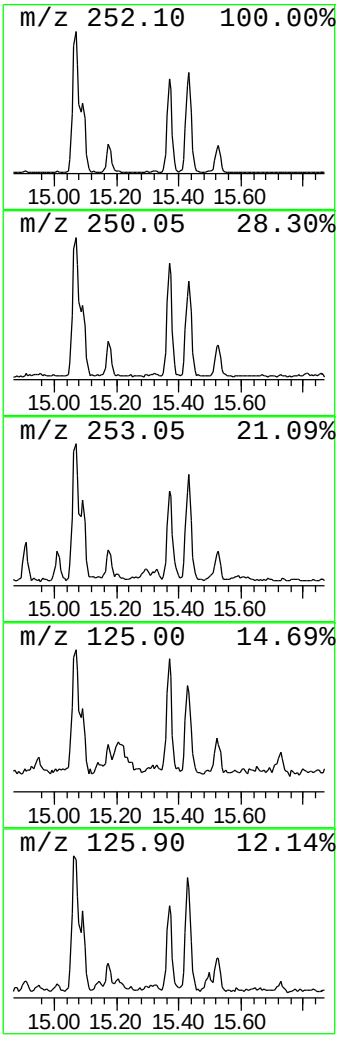
Peak Number 10 Benz[e]acephenanthrylene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.37	3.36 ng	142133	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
2	Benzo[e]pyrene	252	C20H12	000192-97-2	93
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4	Benzo[a]pyrene	252	C20H12	000050-32-8	91
5	Perylene	252	C20H12	000198-55-0	90





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Data File : BF115636.D
Acq On : 17 Jul 2019 21:39
Operator : HP/JU
Sample : K3835-31 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-7(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.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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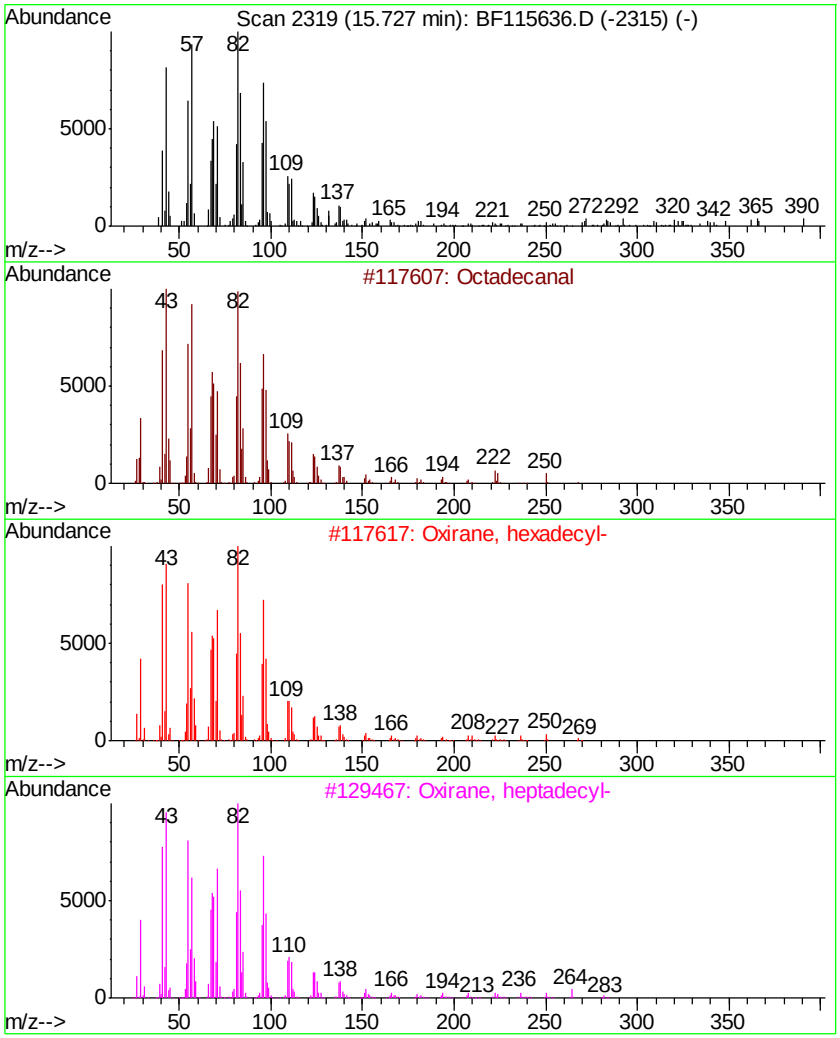
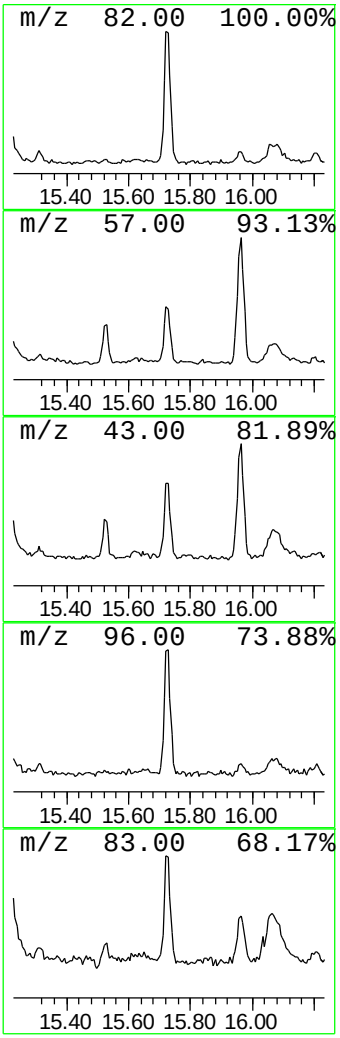
Peak Number 11 Octadecanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.73	6.42 ng	271166	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	91
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	90
4	Tetracosanal	352	C24H48O	057866-08-7	87
5	1,19-Eicosadiene	278	C20H38	014811-95-1	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071719\
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Sample : K3835-31 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-7(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.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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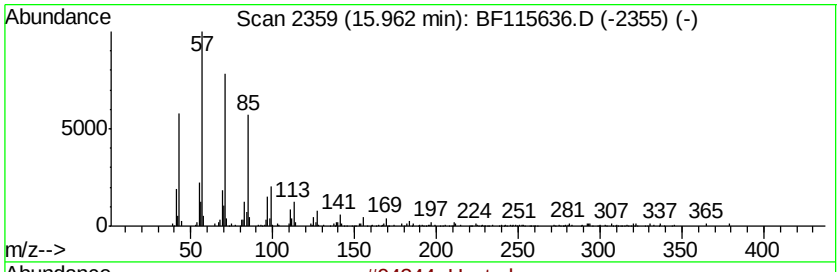
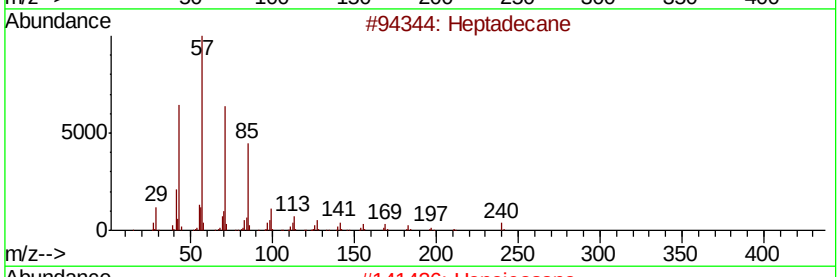
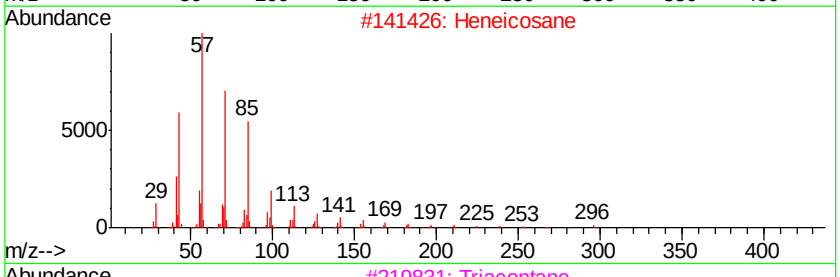
Peak Number 12 Heptadecane Concentration Rank 6

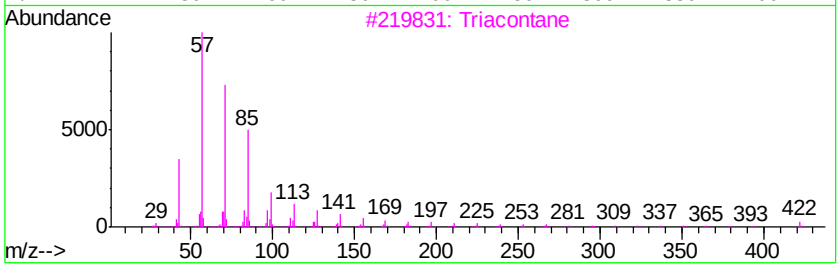
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	6.16 ng	260198	Perylene-d12	15.50

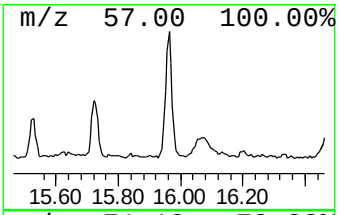
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	91

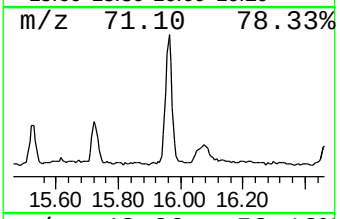


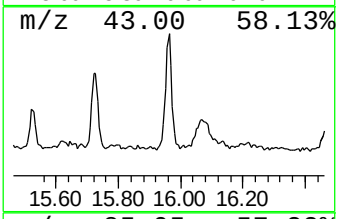


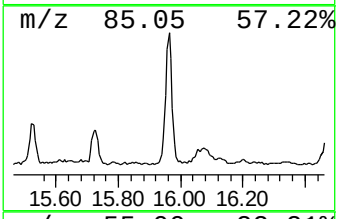


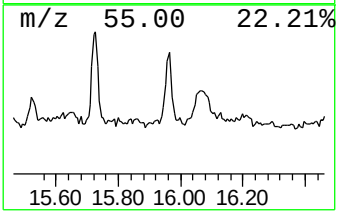












Tentatively Identified Compound (LSC) summary

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Data File : BF115636.D
Acq On : 17 Jul 2019 21:39
Operator : HP/JU
Sample : K3835-31 2X
Misc :
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Instrument :
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SB-7(0-2)

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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...	2.19	8.2	ng	453153	1	6.88	1106970	20.0
unknown6.65	6.65	30.3	ng	1678000	1	6.88	1106970	20.0
n-Hexadecanoic acid	11.92	4.5	ng	236452	4	11.40	1048720	20.0
unknown13.83	13.83	2.0	ng	118996	5	14.03	1171650	20.0
1-Heptacosanol	14.54	3.5	ng	204200	5	14.03	1171650	20.0
Oxirane, hexadecyl-	14.95	3.8	ng	158340	6	15.50	844897	20.0
2-methyloctacosane	15.14	4.6	ng	193394	6	15.50	844897	20.0
3,4:8,9-Dibenzopy...	15.21	10.5	ng	442731	6	15.50	844897	20.0
Benz[e]acephenant...	15.37	3.4	ng	142133	6	15.50	844897	20.0
Octadecanal	15.73	6.4	ng	271166	6	15.50	844897	20.0
Heptadecane	15.96	6.2	ng	260198	6	15.50	844897	20.0