LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102419\
Data File : BF117511.D
Acq On : 24 Oct 2019 15:46
Operator : JU
Sample : K5498-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 191-36-(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	5.357	552	556	576	rBV	529445	691402	87.91%	8.377%
2	5.563	589	591	599	rBV2	7334	10644	1.35%	0.129%
3	6.381	727	730	748	rBV	727773	765527	97.34%	9.275%
4	6.504	748	751	758	rVV	832069	786461	100.00%	9.528%
5	6.569	758	762	767	rVV	27640	36376	4.63%	0.441%
6	6.610	767	769	781	rVB2	9404	13653	1.74%	0.165%
7	6.734	787	790	801	rBV	258282	249843	31.77%	3.027%
8	6.886	813	816	830	rBV	605628	527374	67.06%	6.389%
9	6.998	832	835	846	rVB2	13566	18849	2.40%	0.228%
10	7.298	883	886	893	rBV	422597	428228	54.45%	5.188%
11	7.392	900	902	913	rVB3	4653	9286	1.18%	0.113%
12	7.592	933	936	942	rVB	21770	23184	2.95%	0.281%
13	7.769	962	966	969	rBV	6750	8800	1.12%	0.107%
14	7.816	969	974	984	rVB	14319	20698	2.63%	0.251%
15	8.010	1004	1007	1026	rBV	313274	320218	40.72%	3.880%
16	8.233	1042	1045	1050	rBV	23651	23141	2.94%	0.280%
17	8.286	1052	1054	1063	rVB	26422	27655	3.52%	0.335%
18	8.716	1124	1127	1136	rBB3	14011	16328	2.08%	0.198%
19	9.086	1186	1190	1202	rBV	661970	601571	76.49%	7.288%
20	9.239	1210	1216	1221	rVB2	6229	8436	1.07%	0.102%
21	9.480	1254	1257	1263	rBV	72599	62527	7.95%	0.758%
22	9.763	1302	1305	1309	rBV	412387	333097	42.35%	4.036%
23	9.798	1309	1311	1318	rVB3	12395	13076	1.66%	0.158%
24	10.316	1394	1399	1405	rVB2	6952	10173	1.29%	0.123%
25	10.557	1436	1440	1448	rBV	339472	374759	47.65%	4.540%
26	11.245	1554	1557	1560	rBV	268250	273732	34.81%	3.316%
27	11.274	1560	1562	1567	rVV	81439	76859	9.77%	0.931%
28	11.327	1567	1571	1574	rVB	13758	16190	2.06%	0.196%
29	11.645	1619	1625	1630	rBV4	4750	8202	1.04%	0.099%
30	11.751	1640	1643	1645	rBV2	15876	15300	1.95%	0.185%
31	11.774	1645	1647	1654	rVB3	56841	64916	8.25%	0.786%
32	11.863	1660	1662	1665	rBV2	17717	18225	2.32%	0.221%
33	12.010	1682	1687	1689	rBV3	5839	8096	1.03%	0.098%
34	12.463	1761	1764	1769	rBV	136449	123434	15.69%	1.495%

LSC Area Percent Report

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Acq On : 24 Oct 2019 15:46
Operator : JU
Sample : K5498-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 191-36-(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

35	12.557	1778	1780	1783	rBV2	17349	18279	2.32%	0.221%
36	12.692	1798	1803	1809	rBV	116505	123994	15.77%	1.502%
37	12.827	1823	1826	1831	rBV	467658	396504	50.42%	4.804%
38	13.021	1852	1859	1863	rBV	20630	33433	4.25%	0.405%
39	13.086	1868	1870	1874	rVV	13529	15278	1.94%	0.185%
40	13.127	1874	1877	1884	rVB4	12358	19201	2.44%	0.233%
41	13.251	1896	1898	1903	rVB6	9683	9749	1.24%	0.118%
42	13.298	1903	1906	1911	rVB5	5698	7910	1.01%	0.096%
43	13.727	1977	1979	1988	rVB5	31175	53039	6.74%	0.643%
44	13.862	1999	2002	2003	rBV	32131	29247	3.72%	0.354%
45	13.892	2003	2007	2010	rVV2	322254	364370	46.33%	4.414%
46	13.915	2010	2011	2017	rVB	70538	58105	7.39%	0.704%
47	13.998	2023	2025	2028	rVB3	12063	9682	1.23%	0.117%
48	14.045	2030	2033	2035	rBV2	13460	13435	1.71%	0.163%
49	14.286	2071	2074	2077	rVB	12973	14283	1.82%	0.173%
50	14.351	2082	2085	2088	rBV2	32227	32669	4.15%	0.396%
51	14.651	2133	2136	2141	rVB	43204	46329	5.89%	0.561%
52	14.921	2179	2182	2185	rBV	57036	68915	8.76%	0.835%
53	14.968	2187	2190	2197	rVB	66740	81334	10.34%	0.985%
54	15.027	2198	2200	2203	rVB4	18175	16486	2.10%	0.200%
55	15.209	2228	2231	2235	rBV	37246	47549	6.05%	0.576%
56	15.274	2237	2242	2246	rBV	50033	72231	9.18%	0.875%
57	15.327	2246	2251	2261	rVB2	281161	402327	51.16%	4.874%
58	15.433	2267	2269	2273	rBV4	10014	10967	1.39%	0.133%
59	15.727	2315	2319	2324	rVB2	56569	83116	10.57%	1.007%
60	15.956	2354	2358	2366	rVB10	18817	39318	5.00%	0.476%
61	16.145	2386	2390	2393	rBV6	8627	15668	1.99%	0.190%
62	16.198	2394	2399	2408	rVB2	40753	80794	10.27%	0.979%
63	16.739	2487	2491	2499	rVB3	30564	59259	7.53%	0.718%
64	16.903	2517	2519	2525	rVB7	12912	18269	2.32%	0.221%
65	17.174	2561	2565	2571	rVB2	12111	26063	3.31%	0.316%

Sum of corrected areas: 8254063

LSC Report - Integrated Chromatogram

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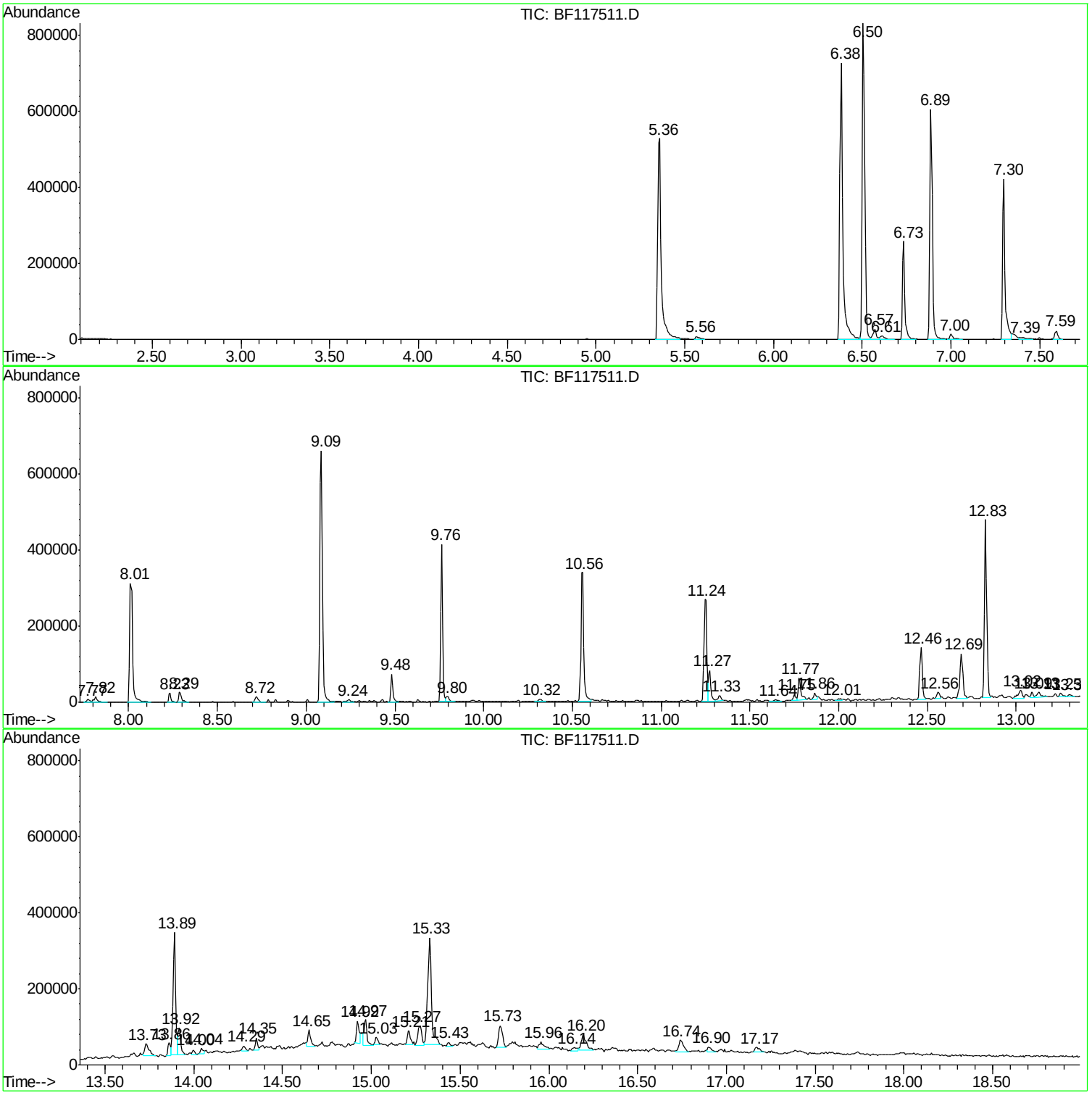
Acq On : 24 Oct 2019 15:46
Operator : JU
Sample : K5498-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
191-36-(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\BF102419\
Data File : BF117511.D
Acq On : 24 Oct 2019 15:46
Operator : JU
Sample : K5498-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 191-36-(0-1)

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

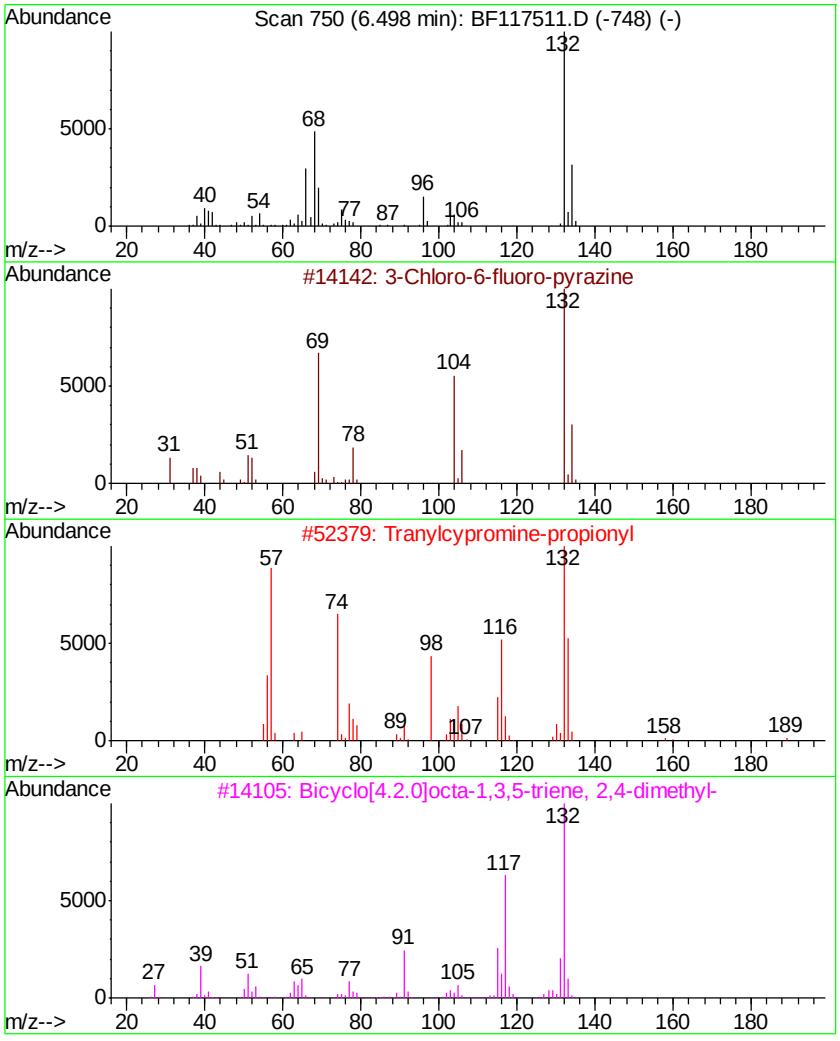
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

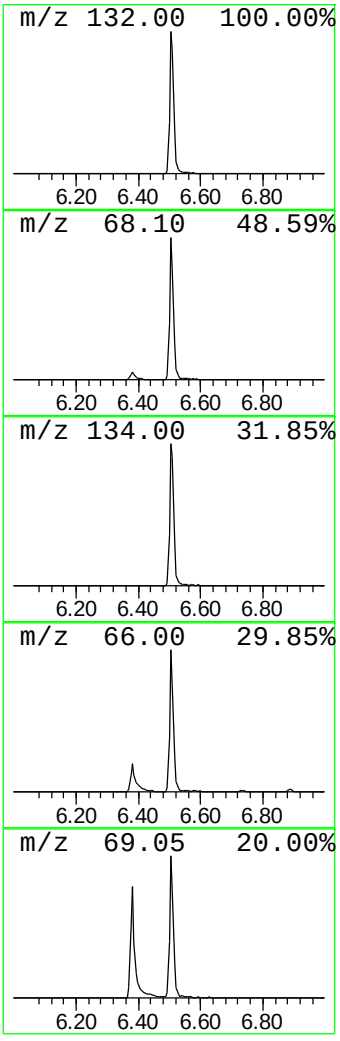
****

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	62.96 ng	786461	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	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102419\
Data File : BF117511.D
Acq On : 24 Oct 2019 15:46
Operator : JU
Sample : K5498-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 191-36-(0-1)

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

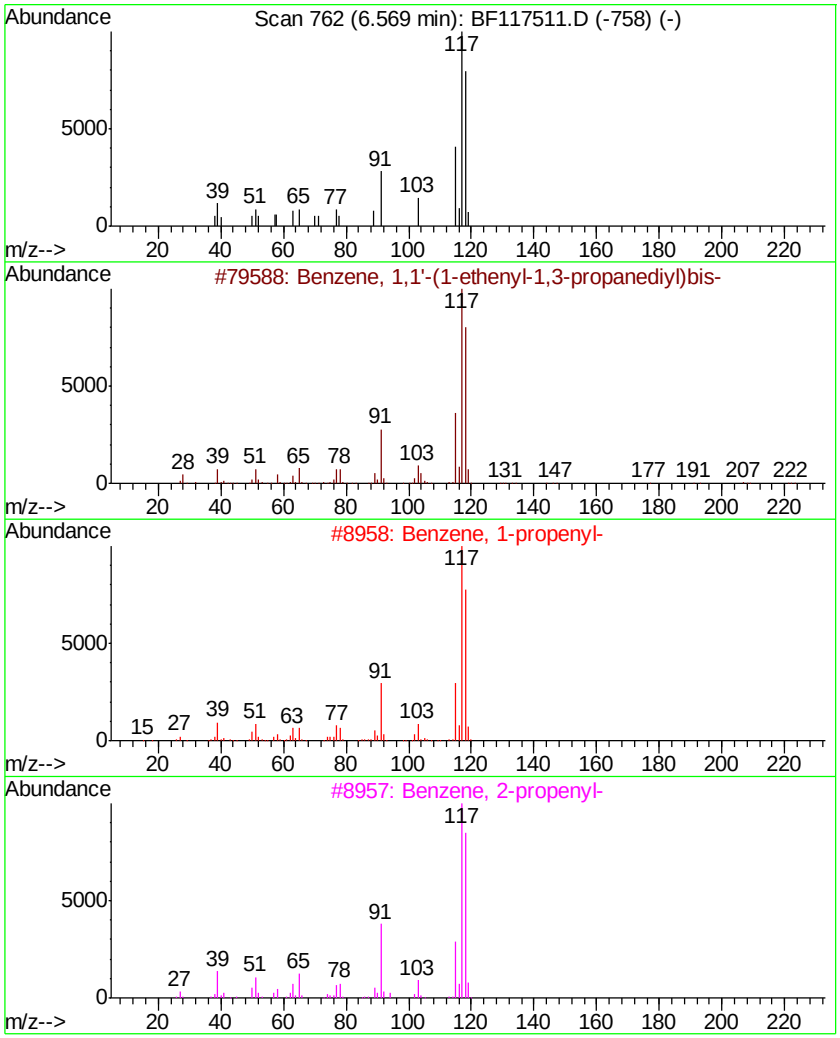
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

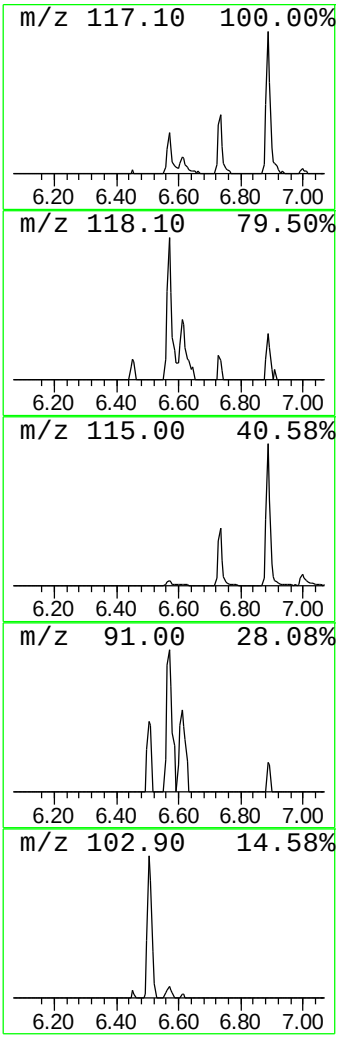
****

Peak Number 2 Benzene, 1,1'-(1-ethenyl-1,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	2.91 ng	36376	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(1-ethenyl-1,3-pro...	222	C17H18	061141-97-7	83
2	Benzene, 1-propenyl-	118	C9H10	000637-50-3	81
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
5	Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	74





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102419\
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Sample : K5498-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 191-36-(0-1)

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

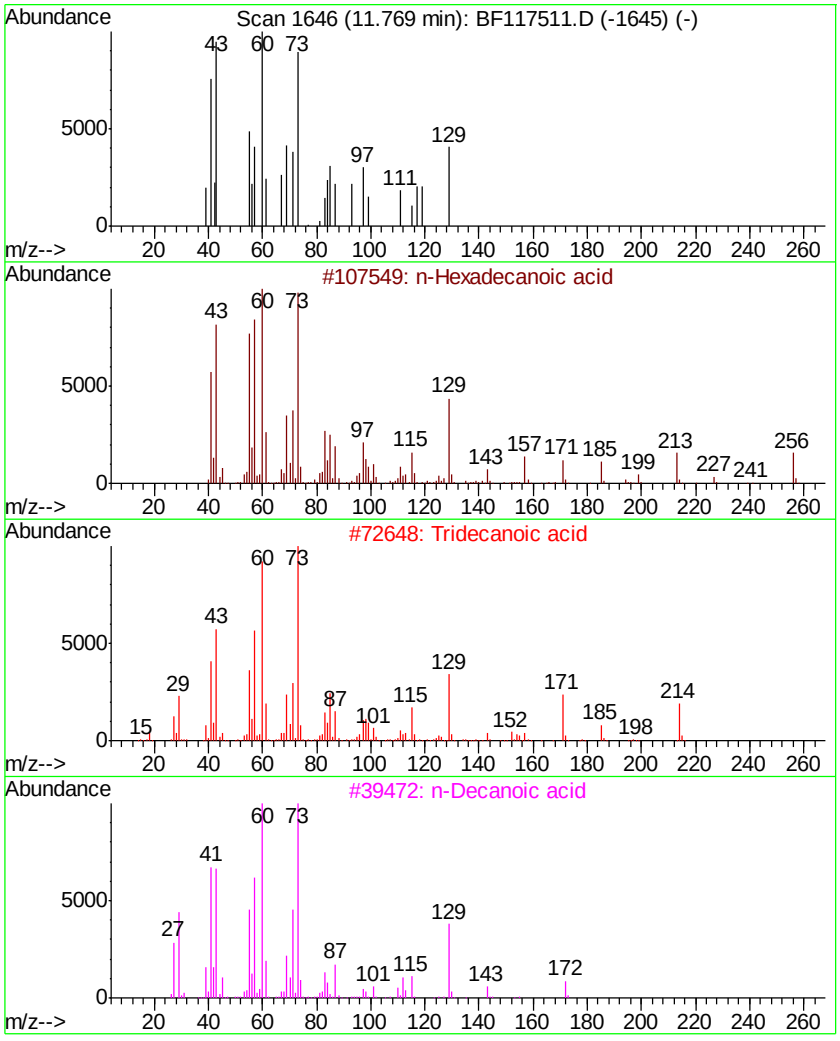
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

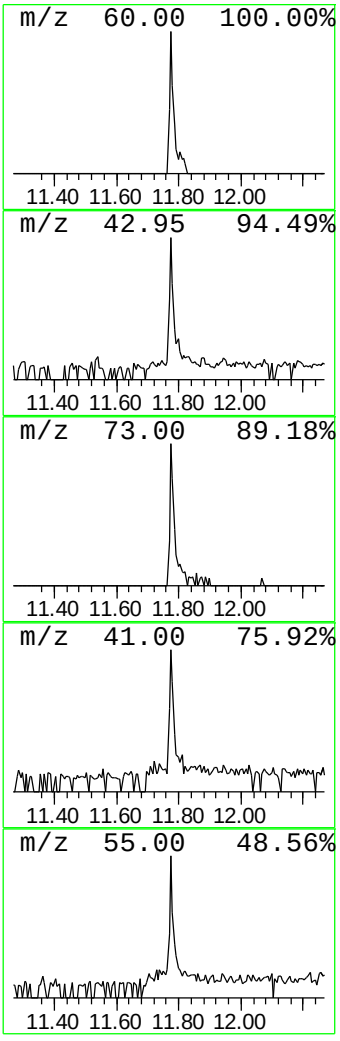
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	4.74 ng	64916	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	59
3	n-Decanoic acid	172	C10H20O2	000334-48-5	59
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	Dodecanoic acid	200	C12H24O2	000143-07-7	38





Library Search Compound Report

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Instrument : BNA_F
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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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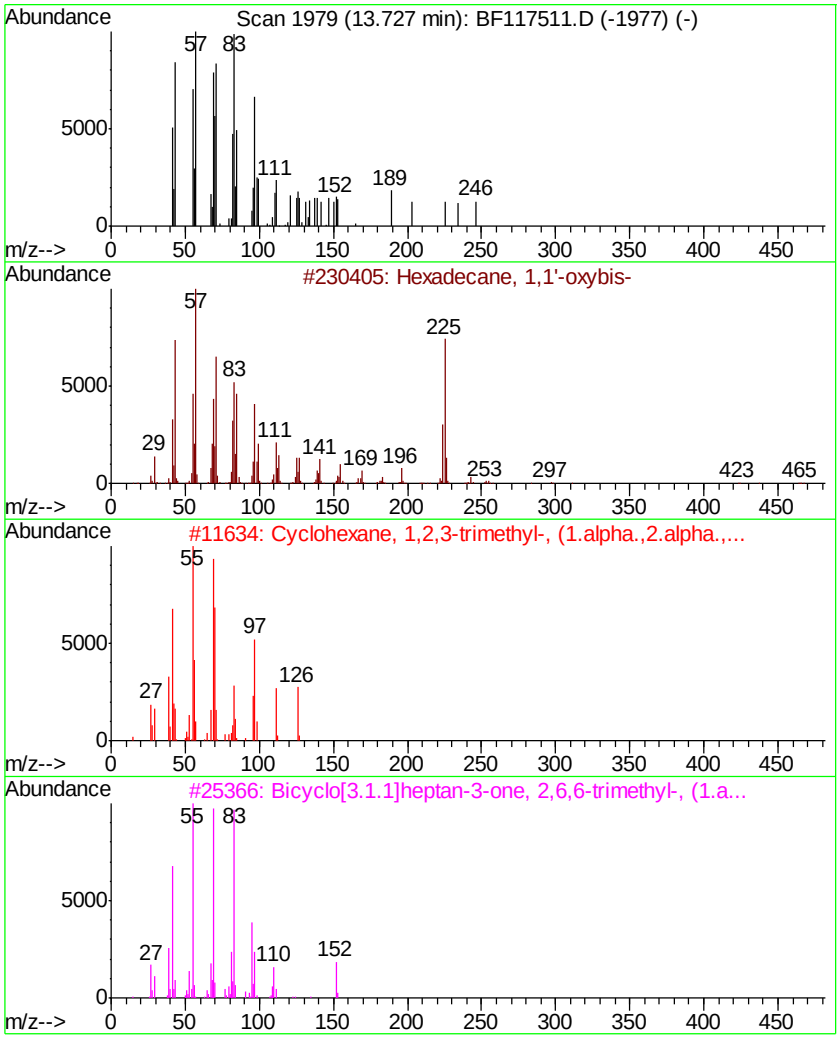
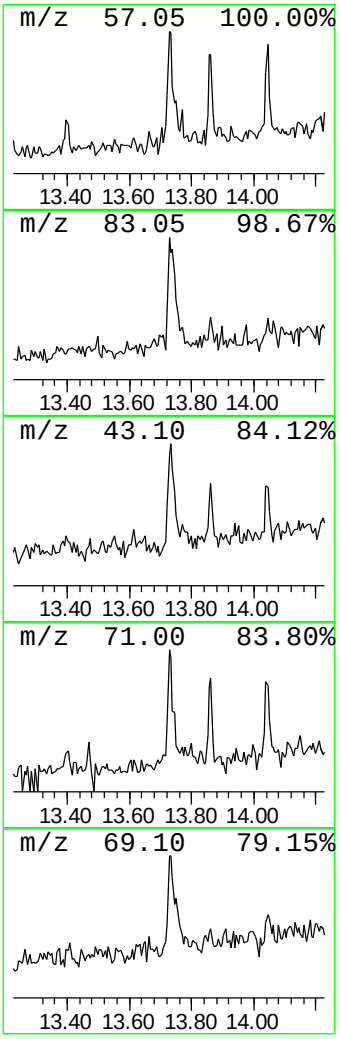
****

Peak Number 5 unknown13.73 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	2.91 ng	53039	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 1,1'-oxybis-	467	C32H66O	004113-12-6	47
2	Cyclohexane, 1,2,3-trimethyl-, (...	126	C9H18	007667-55-2	30
3	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	30
4	2,2,4-Trimethyl-3-hexene	126	C9H18	059643-72-0	25
5	2-Pentene, 3-ethyl-4,4-dimethyl-	126	C9H18	053907-59-8	25





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : 191-36-(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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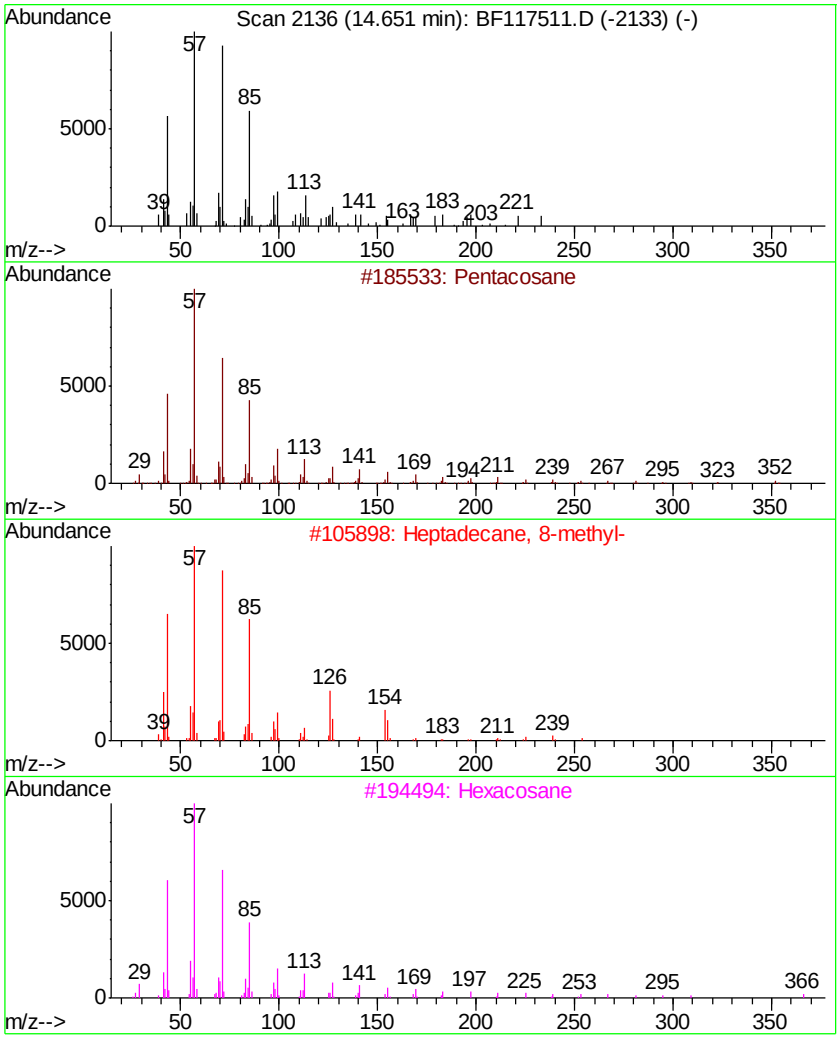
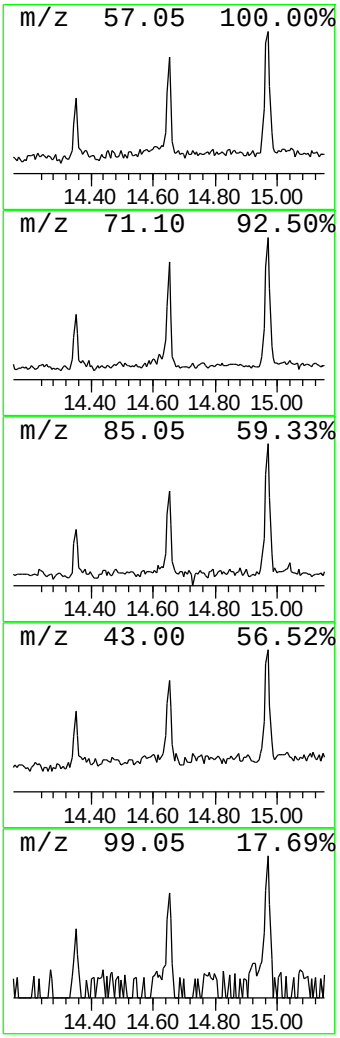
Peak Number 6 Pentacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	2.30 ng	46329	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	90
2	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	86
3	Hexacosane	366	C26H54	000630-01-3	83
4	Octacosane	394	C28H58	000630-02-4	80
5	Pentadecane, 2-methyl-	226	C16H34	001560-93-6	80





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Instrument : BNA_F
ClientSampleId : 191-36-(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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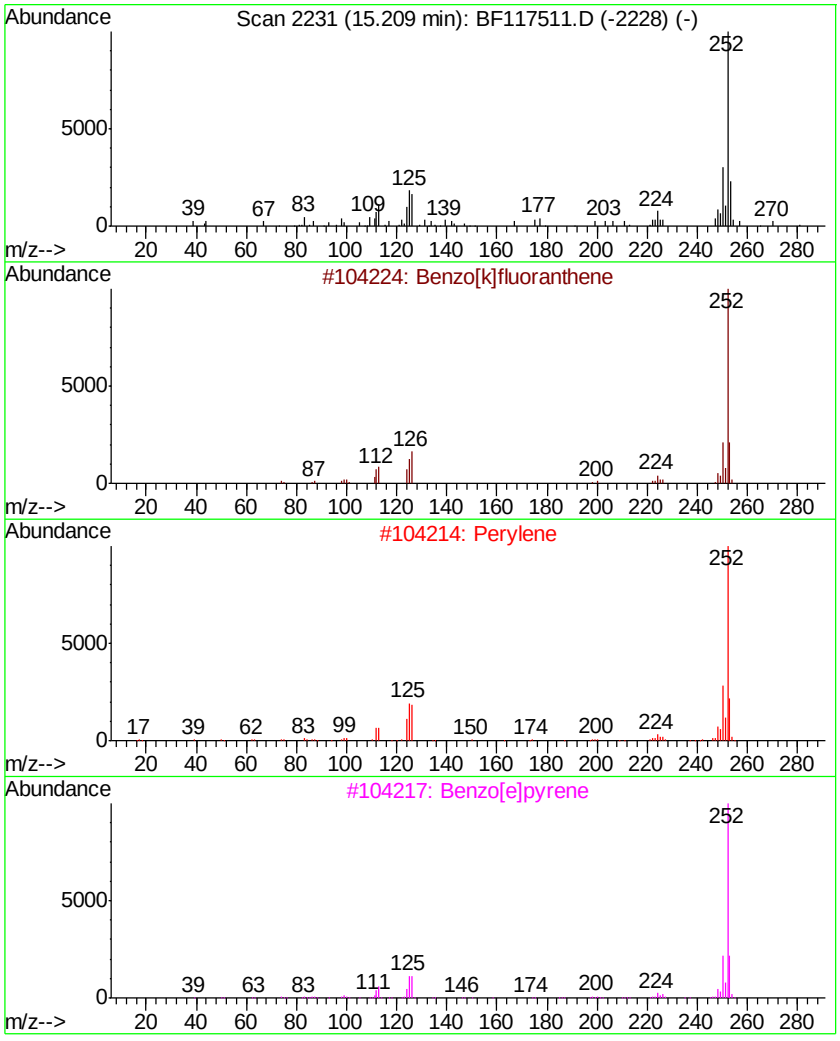
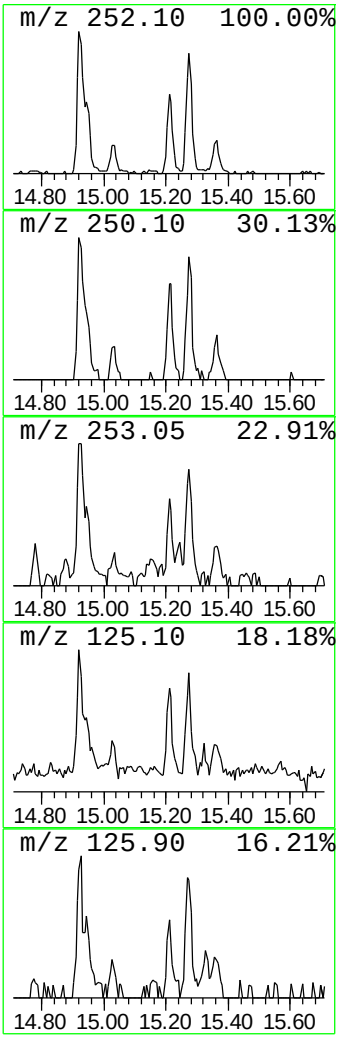
Peak Number 7 Perylene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.21	2.36 ng	47549	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
2	Perylene	252	C20H12	000198-55-0	95
3	Benzo[e]pyrene	252	C20H12	000192-97-2	94
4	Benzo[a]pyrene	252	C20H12	000050-32-8	93
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102419\
Data File : BF117511.D
Acq On : 24 Oct 2019 15:46
Operator : JU
Sample : K5498-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 191-36-(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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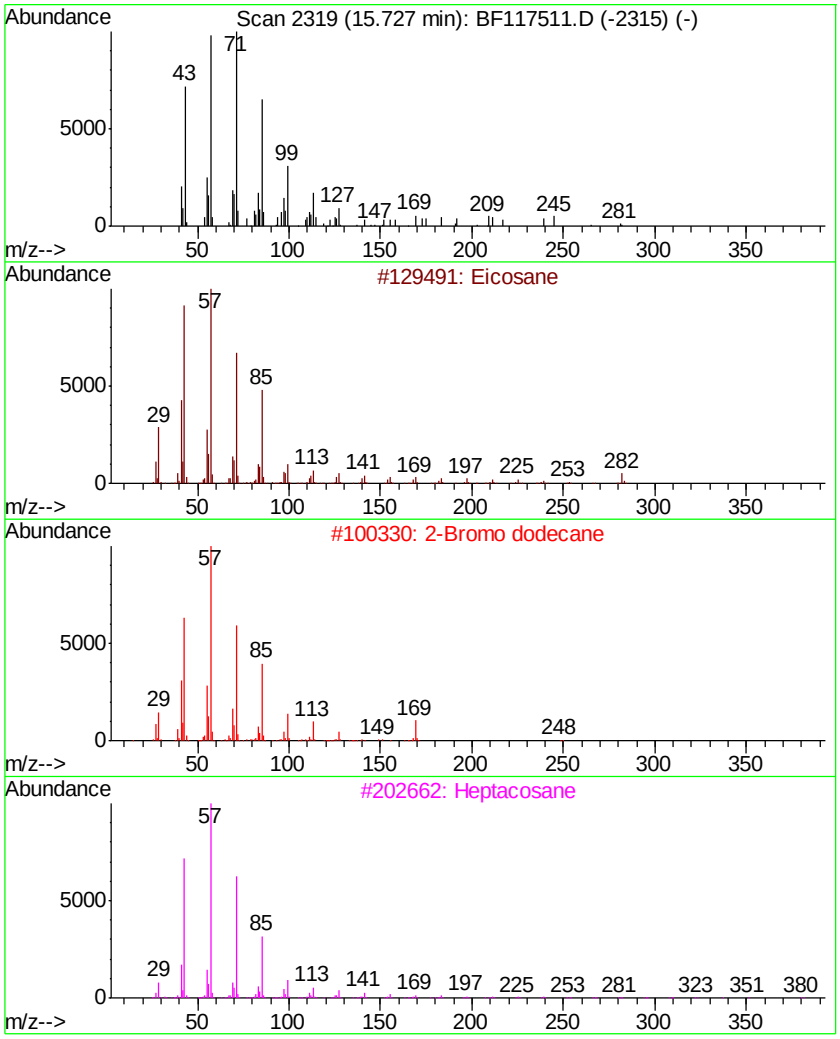
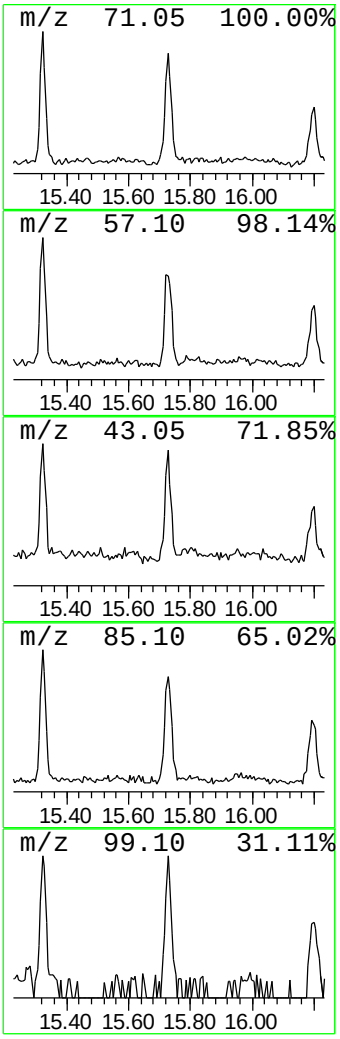
Peak Number 8 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.73	4.13 ng	83116	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	2-Bromo dodecane	248	C12H25Br	013187-99-0	86
3	Heptacosane	380	C27H56	000593-49-7	80
4	Hexacosane	366	C26H54	000630-01-3	74
5	Octacosane	394	C28H58	000630-02-4	72





Library Search Compound Report

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Data File : BF117511.D
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ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 191-36-(0-1)

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

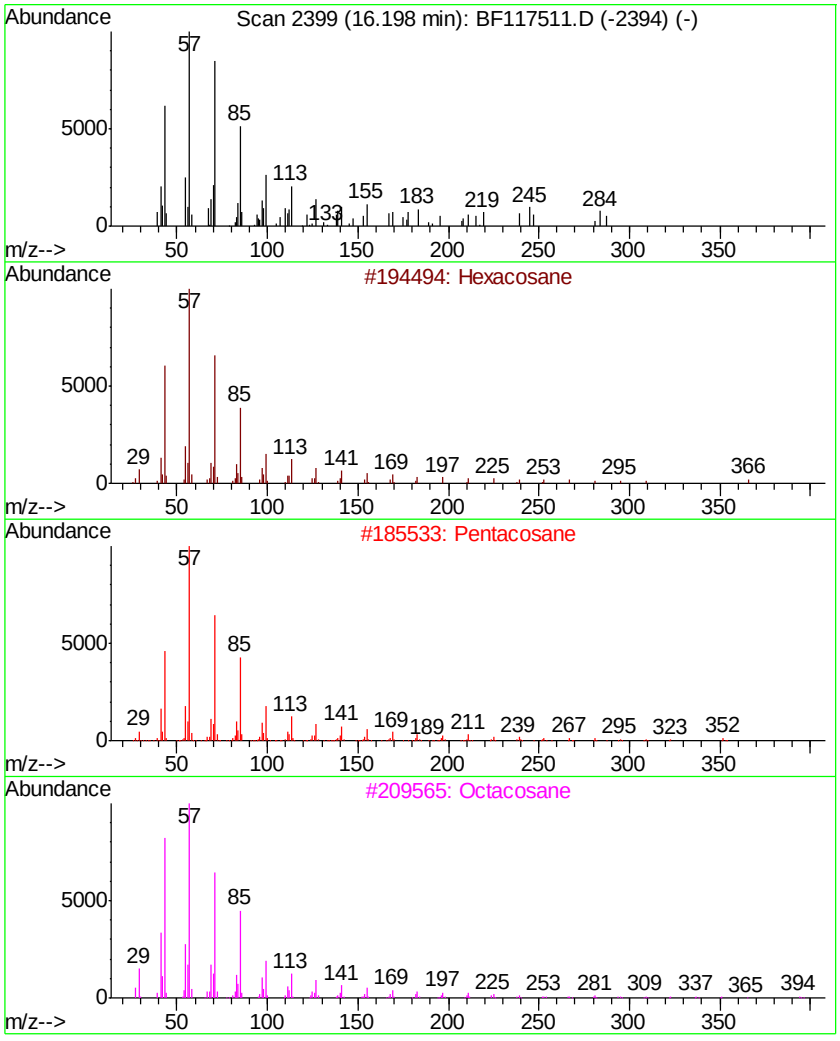
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

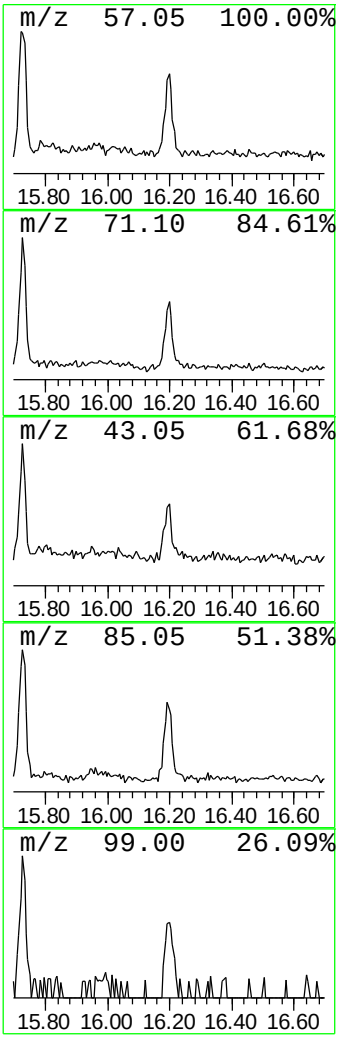
****

Peak Number 9 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.20	4.02 ng	80794	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	83
2	Pentacosane	352	C25H52	000629-99-2	80
3	Octacosane	394	C28H58	000630-02-4	74
4	Tetracosane	338	C24H50	000646-31-1	72
5	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102419\
Data File : BF117511.D
Acq On : 24 Oct 2019 15:46
Operator : JU
Sample : K5498-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 191-36-(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
unknown6.50	6.50	63.0	ng	786461	1	6.73	249843	20.0
Benzene, 1,1'-(1-...	6.57	2.9	ng	36376	1	6.73	249843	20.0
n-Hexadecanoic acid	11.77	4.7	ng	64916	4	11.24	273732	20.0
unknown13.73	13.73	2.9	ng	53039	5	13.89	364370	20.0
Pentacosane	14.65	2.3	ng	46329	6	15.33	402327	20.0
Perylene	15.21	2.4	ng	47549	6	15.33	402327	20.0
Eicosane	15.73	4.1	ng	83116	6	15.33	402327	20.0
Hexacosane	16.20	4.0	ng	80794	6	15.33	402327	20.0