LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122819\
Data File : BF118379.D
Acq On : 28 Dec 2019 21:46
Operator : JU
Sample : K6443-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PH-3

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	4.422	394	397	417	rBV	70689	120336	4.22%	0.448%
2	5.051	500	504	516	rBV	397470	490679	17.22%	1.828%
3	5.469	571	575	584	rBV	1913924	1966847	69.03%	7.327%
4	6.487	744	748	767	rBV	2320426	2191800	76.93%	8.165%
5	6.622	767	771	774	rBV	2858330	2313707	81.21%	8.620%
6	6.851	807	810	817	rBV	756462	623420	21.88%	2.323%
7	7.004	833	836	850	rVB	1944292	1833074	64.34%	6.829%
8	7.416	902	906	918	rBV	1477570	1354390	47.54%	5.046%
9	8.139	1026	1029	1037	rBV	809757	800801	28.11%	2.983%
10	8.857	1148	1151	1157	rBV	48563	49967	1.75%	0.186%
11	8.957	1164	1168	1171	rBV	43108	40211	1.41%	0.150%
12	9.216	1208	1212	1223	rBV	3422470	2849198	100.00%	10.615%
13	9.557	1267	1270	1273	rBV	29352	32903	1.15%	0.123%
14	9.610	1277	1279	1287	rVB	145146	169596	5.95%	0.632%
15	9.763	1302	1305	1309	rVB	55588	52651	1.85%	0.196%
16	9.898	1323	1328	1338	rBV	1118384	993485	34.87%	3.701%
17	10.692	1459	1463	1478	rBV	1835508	1778697	62.43%	6.626%
18	10.810	1478	1483	1490	rVB4	53043	84067	2.95%	0.313%
19	11.245	1553	1557	1560	rBV2	32986	32562	1.14%	0.121%
20	11.392	1578	1582	1585	rBV	1080887	947156	33.24%	3.529%
21	11.416	1585	1586	1591	rVB	137670	96922	3.40%	0.361%
22	11.916	1663	1671	1679	rBV2	257705	397536	13.95%	1.481%
23	12.010	1684	1687	1689	rVV2	73427	85785	3.01%	0.320%
24	12.033	1689	1691	1696	rVB	56750	52138	1.83%	0.194%
25	12.080	1696	1699	1703	rBV	32820	36438	1.28%	0.136%
26	12.192	1715	1718	1722	rBV2	27950	33930	1.19%	0.126%
27	12.445	1758	1761	1764	rBV	78194	84339	2.96%	0.314%
28	12.474	1764	1766	1770	rVV3	53621	75091	2.64%	0.280%
29	12.539	1774	1777	1780	rVV4	26152	37113	1.30%	0.138%
30	12.610	1786	1789	1794	rBV	210751	202036	7.09%	0.753%
31	12.704	1802	1805	1809	rBV2	77064	91827	3.22%	0.342%
32	12.839	1823	1828	1835	rBV	234030	289994	10.18%	1.080%
33	12.898	1835	1838	1841	rVB	36243	37066	1.30%	0.138%
34	12.980	1848	1852	1855	rBV	3120694	2578964	90.52%	9.608%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
ClientSampleId : PH-3

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	13.063	1862	1866	1871	rBV4	34405	56374	1.98%	0.210%
36	13.168	1878	1884	1887	rBV	63137	103961	3.65%	0.387%
37	13.204	1887	1890	1894	rBV2	30449	43478	1.53%	0.162%
38	13.274	1899	1902	1908	rVB2	55586	66751	2.34%	0.249%
39	13.368	1915	1918	1921	rBV	47792	41976	1.47%	0.156%
40	13.398	1921	1923	1926	rVV	43208	39126	1.37%	0.146%
41	13.545	1945	1948	1951	rBV3	37305	38183	1.34%	0.142%
42	13.686	1970	1972	1976	rVB	36974	38586	1.35%	0.144%
43	13.745	1979	1982	1985	rBV2	26010	33905	1.19%	0.126%
44	13.798	1986	1991	1993	rBV3	43335	58598	2.06%	0.218%
45	13.880	2001	2005	2011	rBV4	197024	319967	11.23%	1.192%
46	14.045	2028	2033	2036	rBV2	938367	986971	34.64%	3.677%
47	14.068	2036	2037	2041	rVB	132889	107963	3.79%	0.402%
48	14.192	2056	2058	2060	rBV	40573	38303	1.34%	0.143%
49	14.433	2097	2099	2103	rVB	63216	54511	1.91%	0.203%
50	14.498	2108	2110	2114	rBV3	74157	91608	3.22%	0.341%
51	14.810	2161	2163	2165	rVB	62710	44042	1.55%	0.164%
52	14.886	2173	2176	2181	rVB	117739	122664	4.31%	0.457%
53	15.104	2209	2213	2216	rBV	118954	186654	6.55%	0.695%
54	15.151	2219	2221	2227	rVB3	109785	122804	4.31%	0.457%
55	15.410	2262	2265	2269	rVB	102865	109307	3.84%	0.407%
56	15.474	2272	2276	2282	rBV	143100	196222	6.89%	0.731%
57	15.539	2282	2287	2294	rBV	763716	1035806	36.35%	3.859%
58	15.980	2359	2362	2366	rVB2	60757	79988	2.81%	0.298%

Sum of corrected areas: 26842474

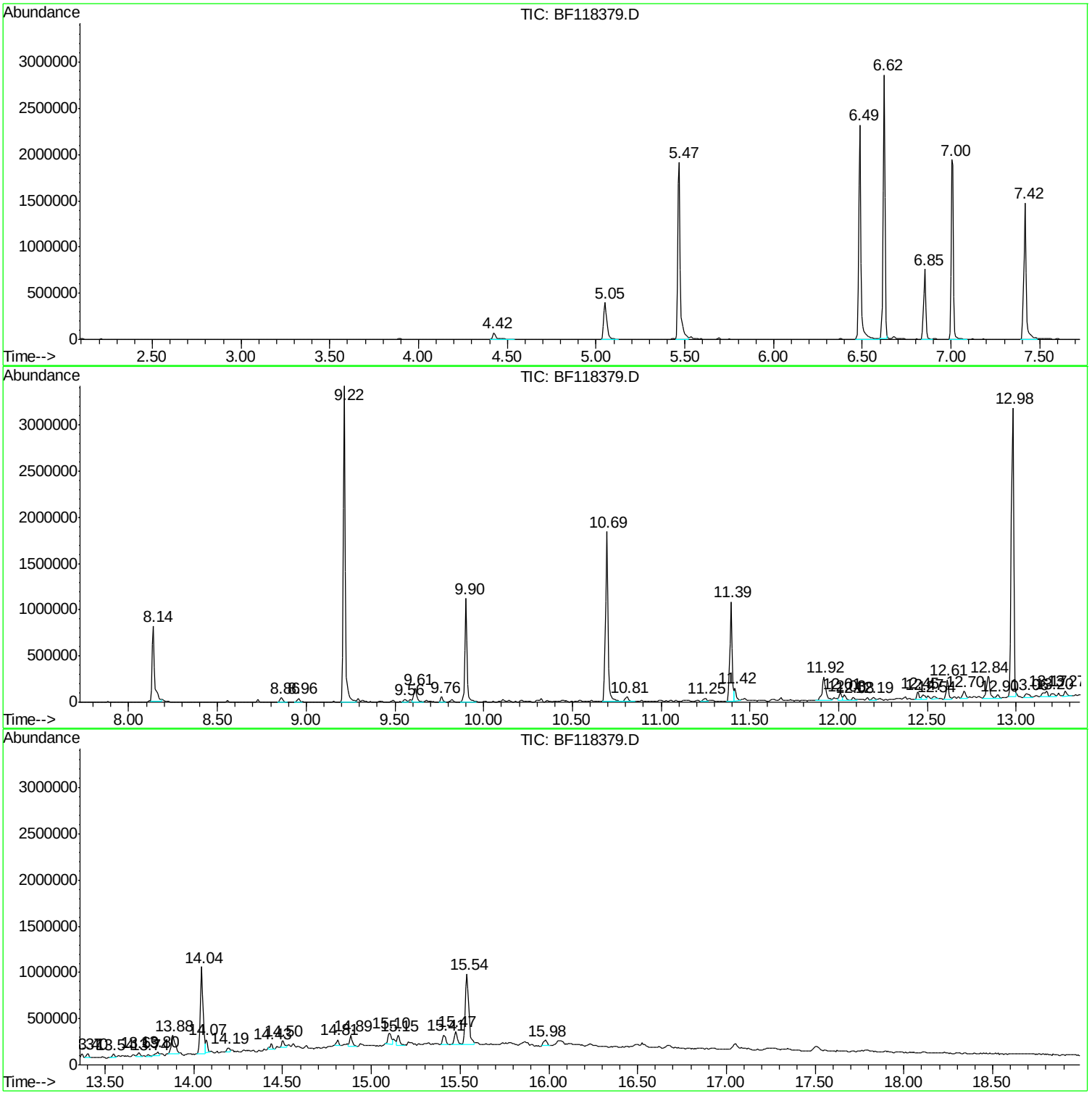
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122819\
Data File : BF118379.D
Acq On : 28 Dec 2019 21:46
Operator : JU
Sample : K6443-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PH-3

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122819\
Data File : BF118379.D
Acq On : 28 Dec 2019 21:46
Operator : JU
Sample : K6443-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PH-3

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

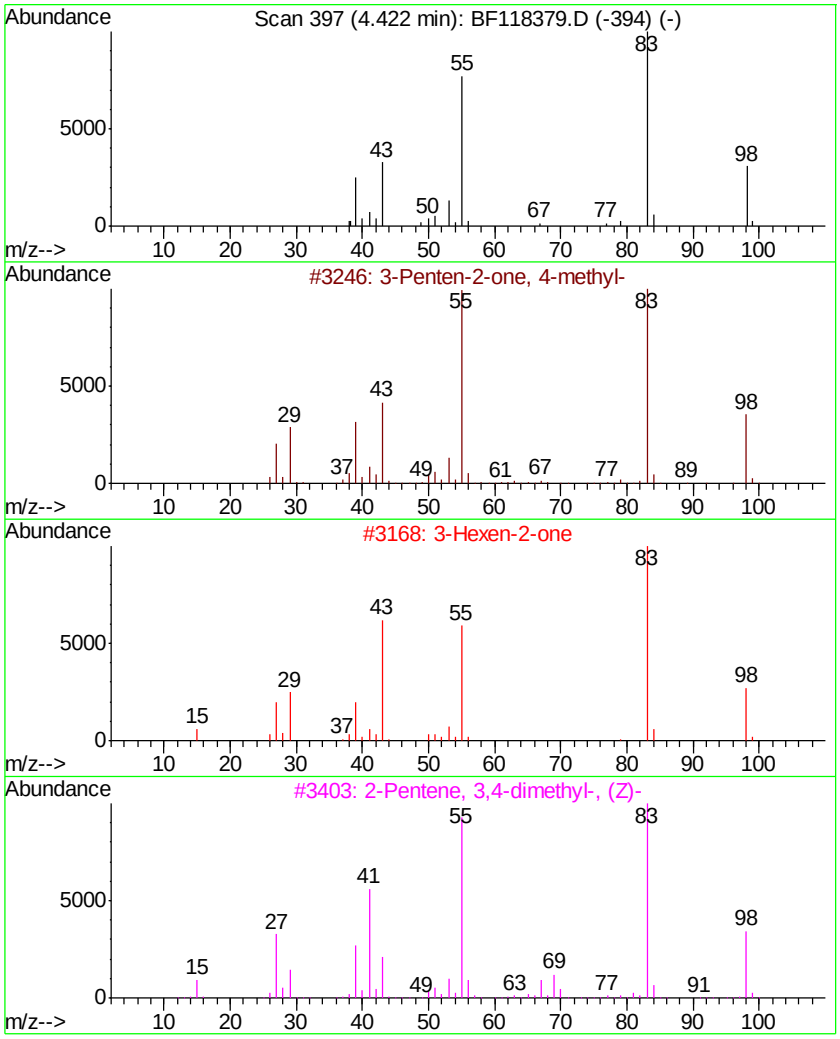
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

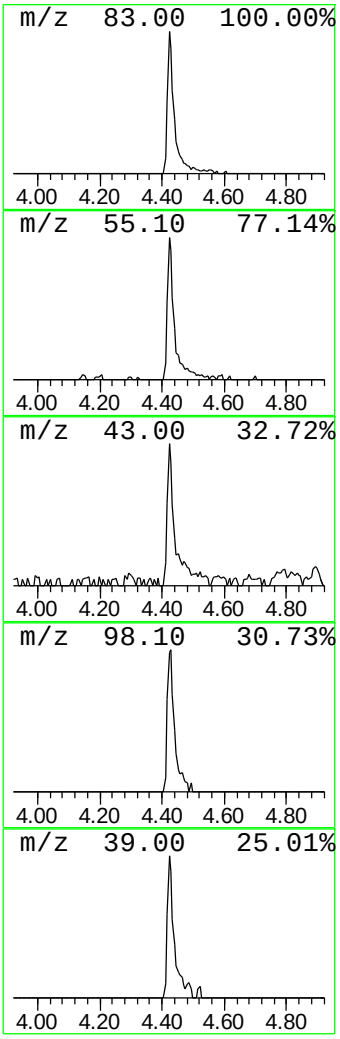
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.42	3.86 ng	120336	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	90
4	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	90
5	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122819\
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Acq On : 28 Dec 2019 21:46
Operator : JU
Sample : K6443-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PH-3

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

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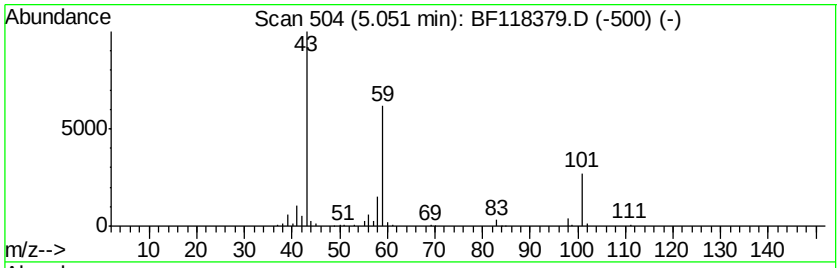
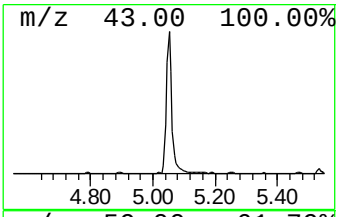
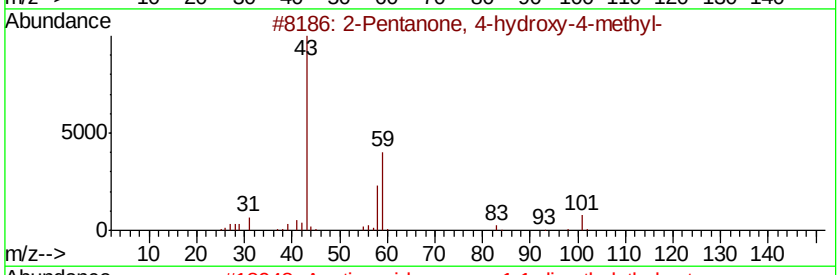
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

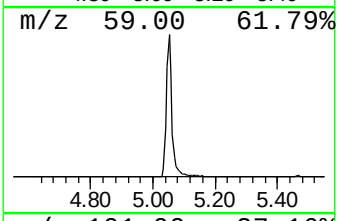
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	15.74 ng	490679	1,4-Dichlorobenzene-d4	6.85

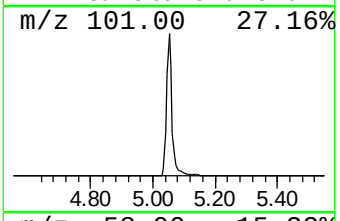
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9

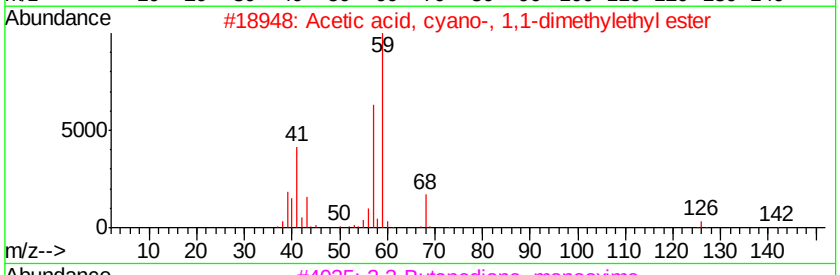


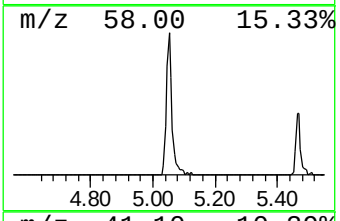


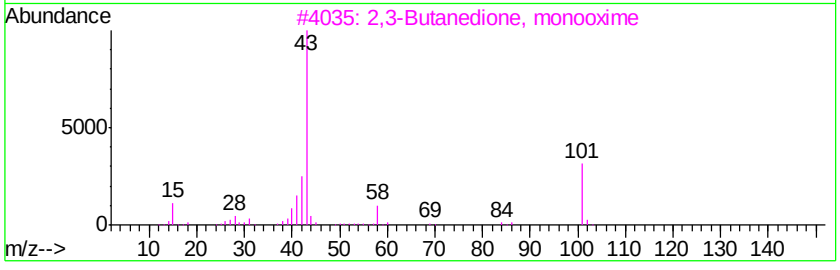


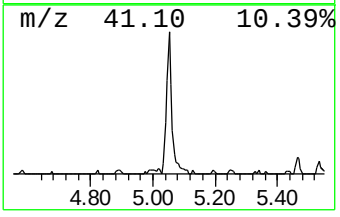












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Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PH-3

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

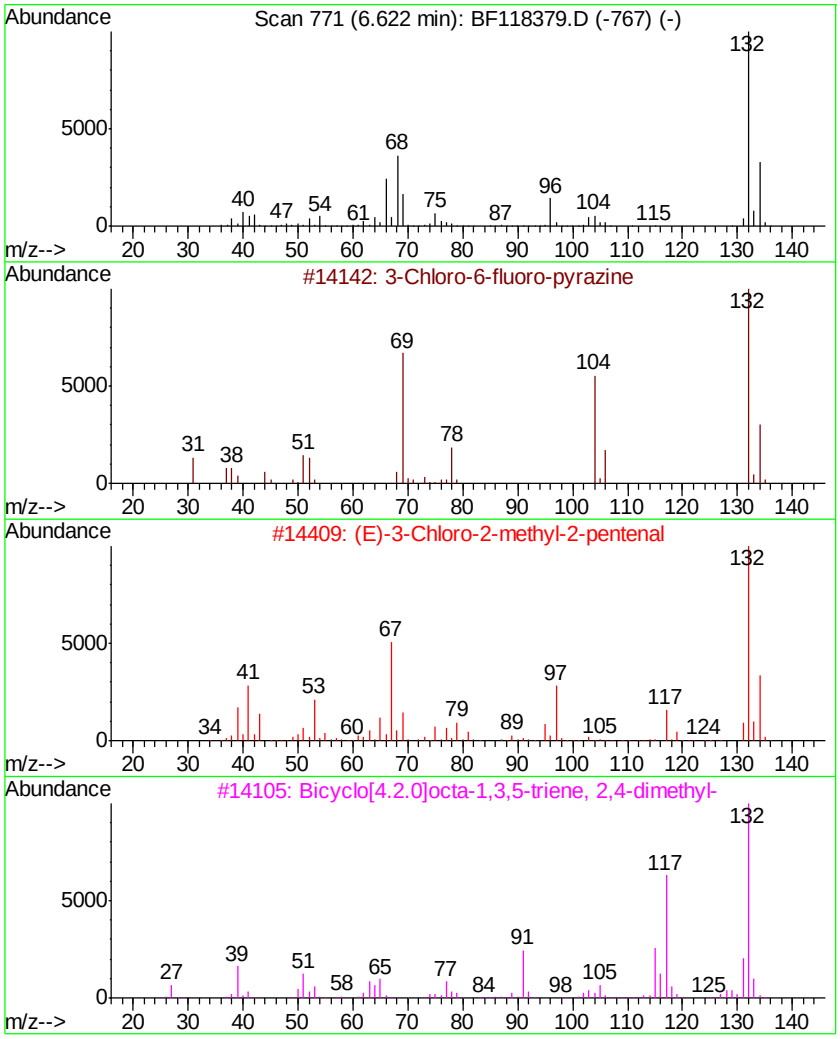
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

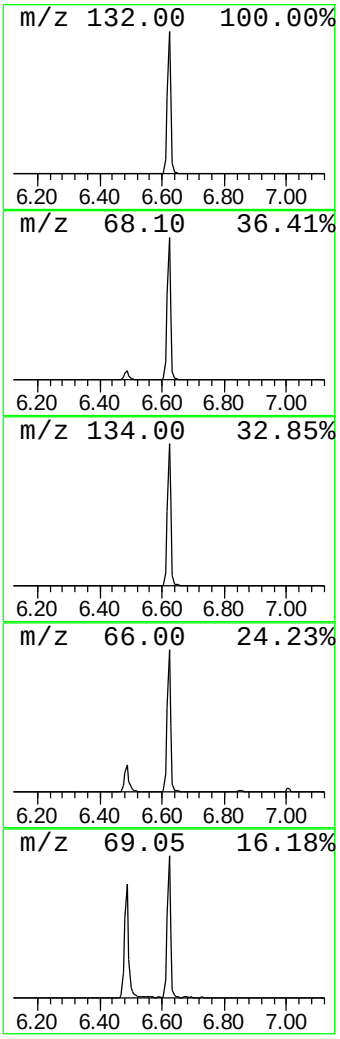
****

Peak Number 3 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	74.23 ng	2313710	1,4-Dichlorobenzene-d4	6.85

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	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	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9





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

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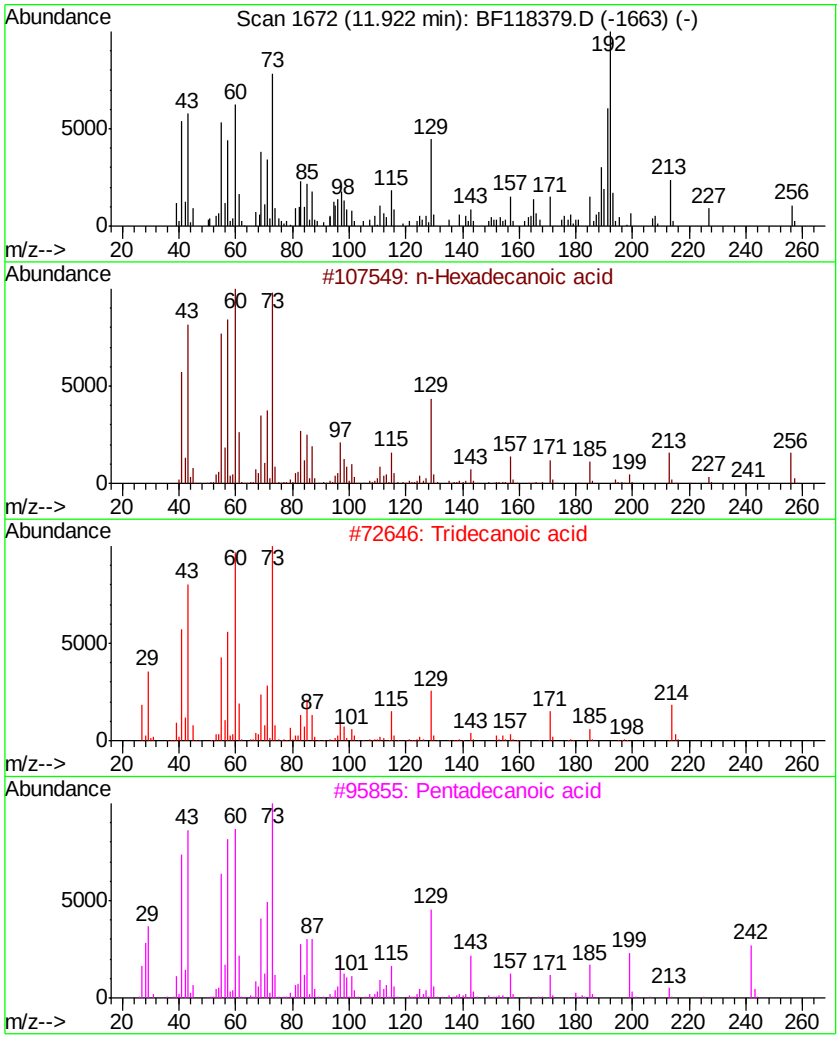
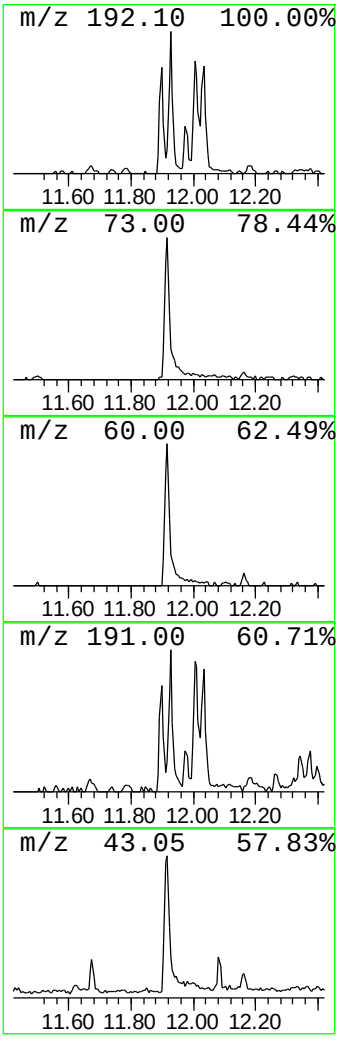
Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	8.39 ng	397536	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	81
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	n-Decanoic acid	172	C10H20O2	000334-48-5	68
5	Nonanoic acid	158	C9H18O2	000112-05-0	30





Library Search Compound Report

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Misc :
ALS Vial : 24 Sample Multiplier: 1

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

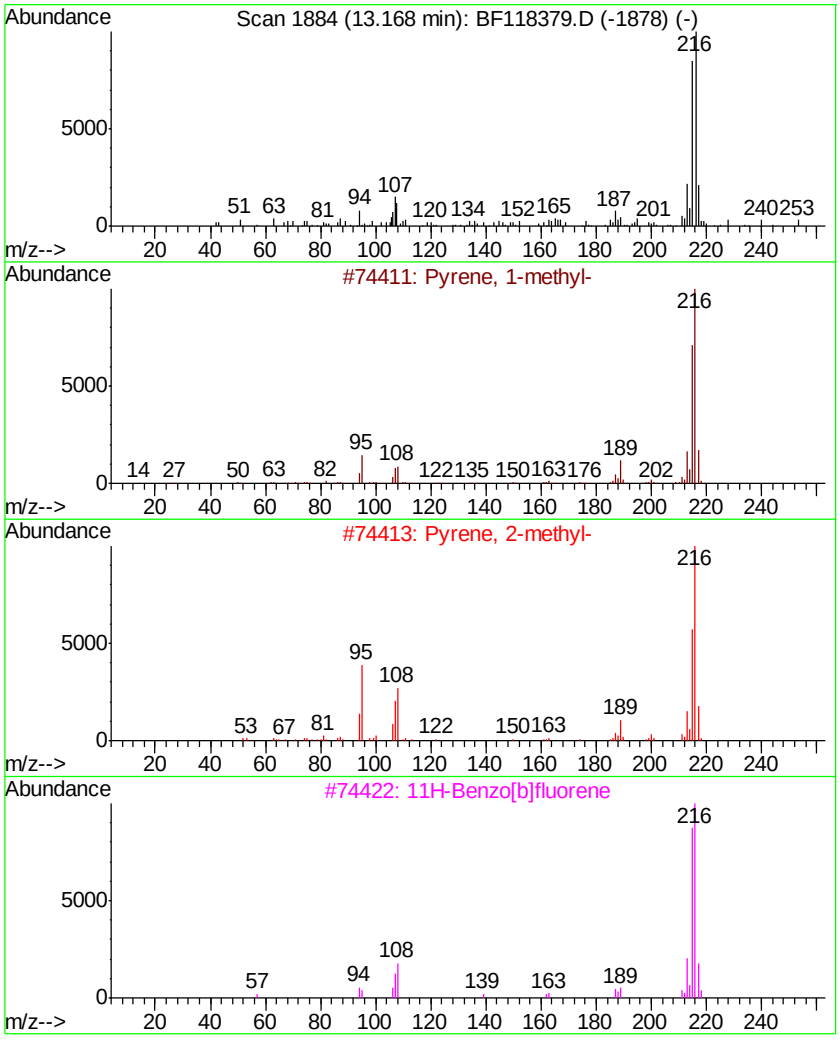
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

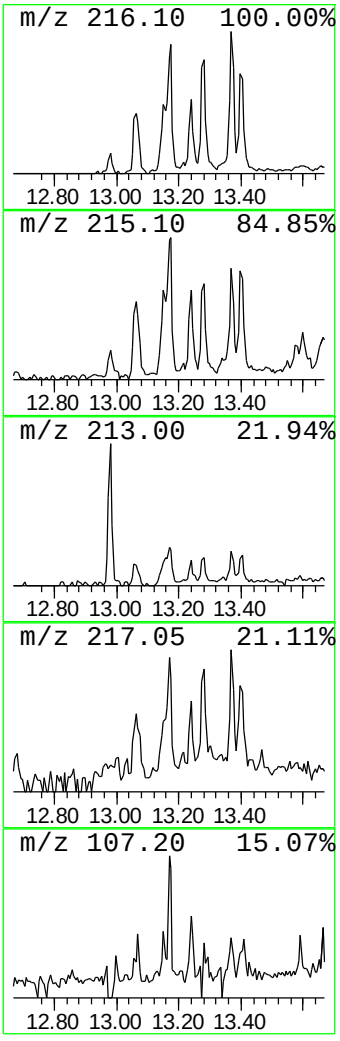
****

Peak Number 6 Pyrene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.17	2.11 ng	103961	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	96
2	Pyrene, 2-methyl-	216	C17H12	003442-78-2	93
3	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	91
5	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	81





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122819\
Data File : BF118379.D
Acq On : 28 Dec 2019 21:46
Operator : JU
Sample : K6443-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PH-3

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

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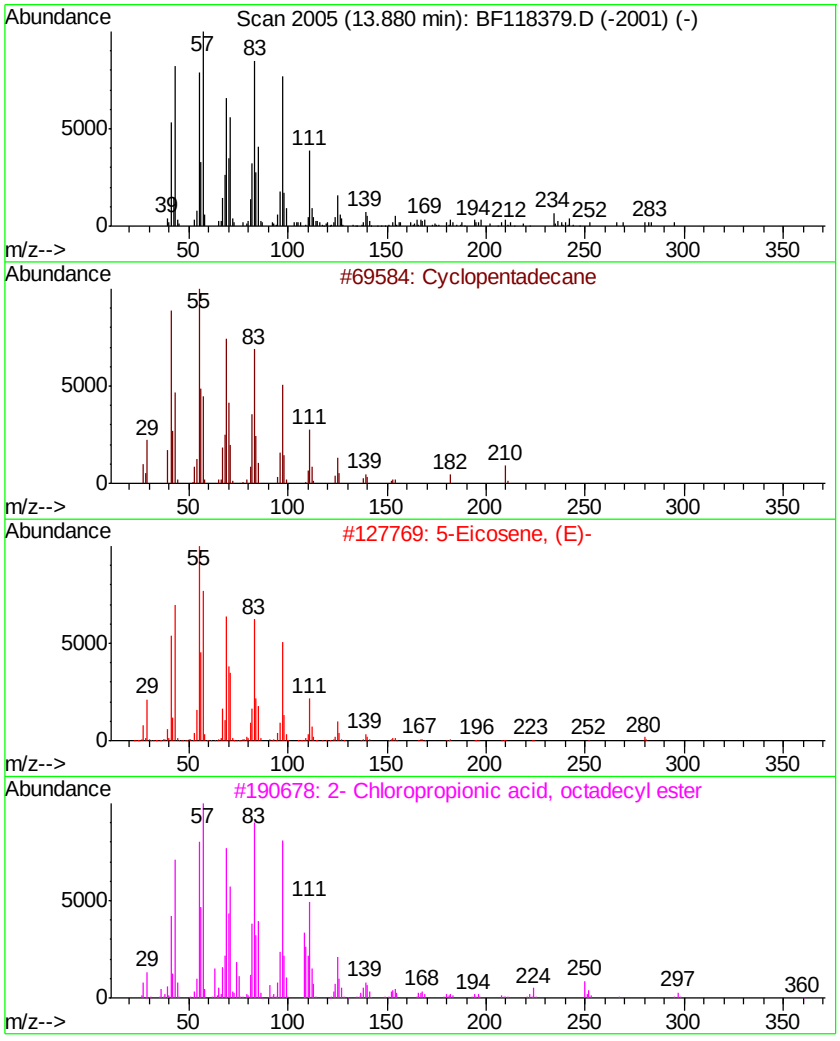
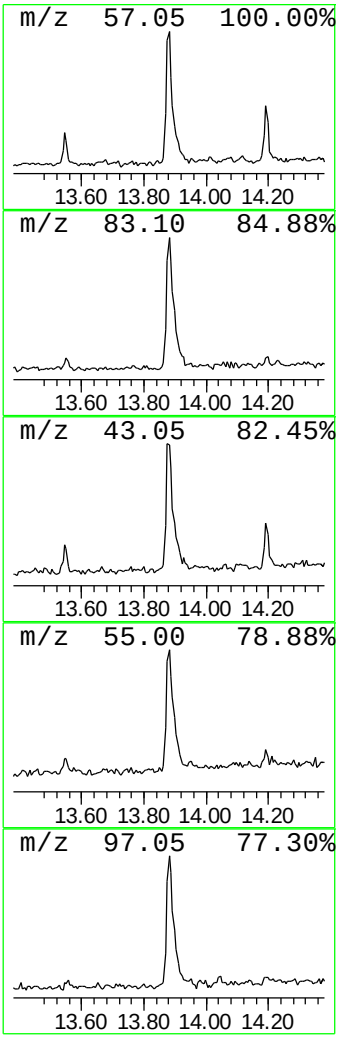
Peak Number 7 Cyclopentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	6.48 ng	319967	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	97
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	93
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
4	1-Heneicosanol	312	C21H44O	015594-90-8	90
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122819\
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Operator : JU
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Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PH-3

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

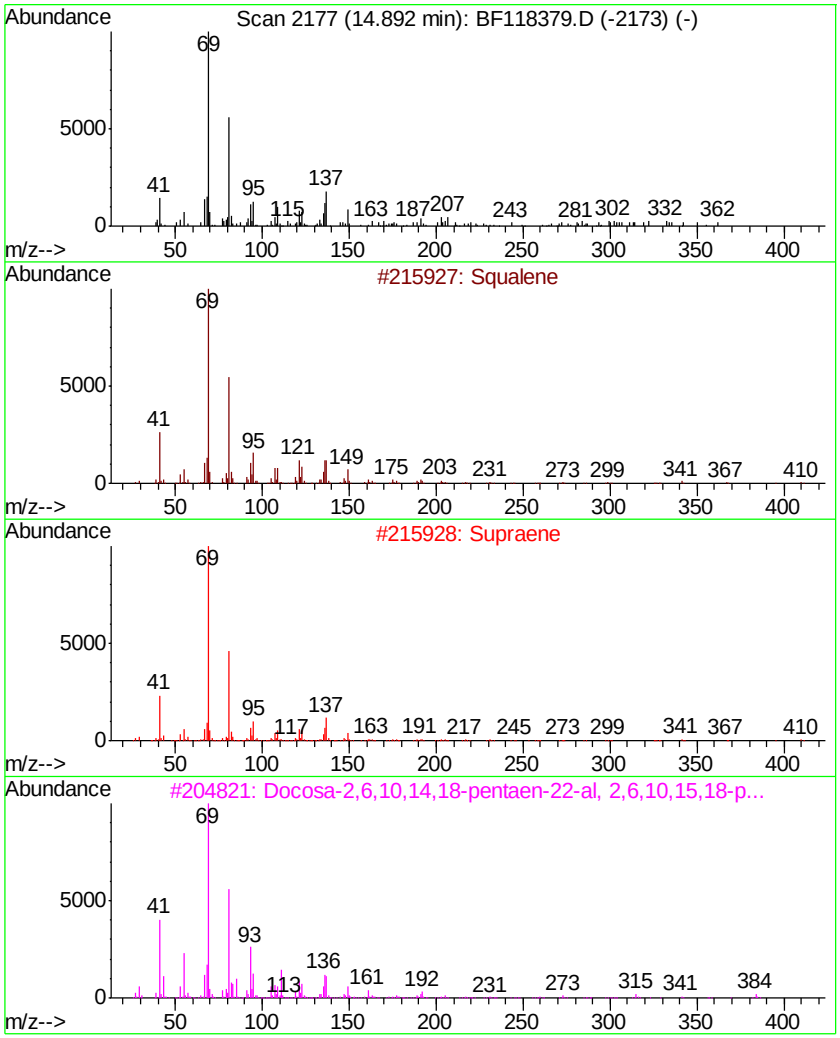
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

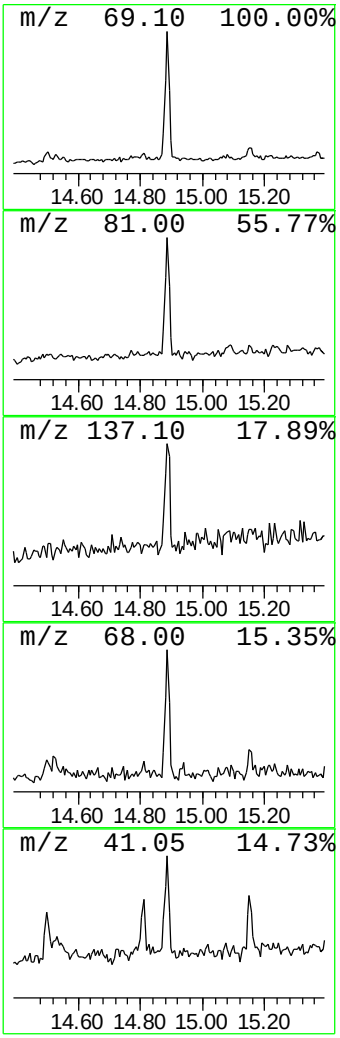
****

Peak Number 8 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	2.37 ng	122664	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	87
2	Supraene	410	C30H50	007683-64-9	87
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	80
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122819\
Data File : BF118379.D
Acq On : 28 Dec 2019 21:46
Operator : JU
Sample : K6443-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PH-3

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

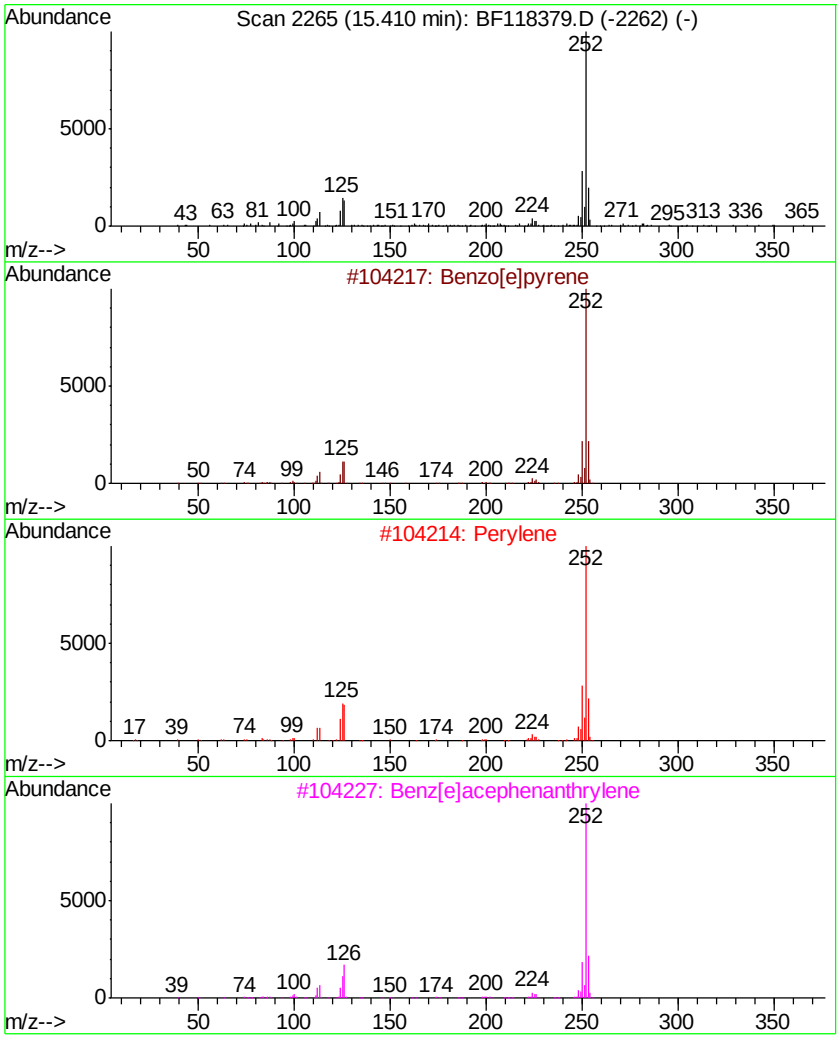
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

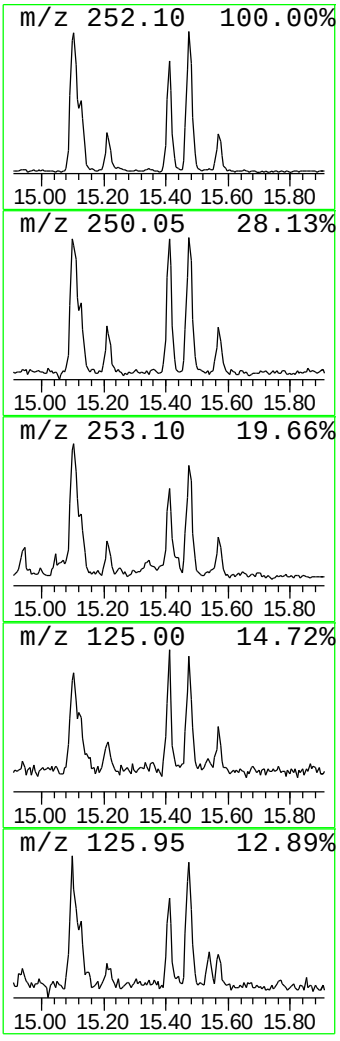
****

Peak Number 9 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.41	2.11 ng	109307	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	98
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	98
4	Benzo[a]pyrene	252	C20H12	000050-32-8	98
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF122819\
Data File : BF118379.D
Acq On : 28 Dec 2019 21:46
Operator : JU
Sample : K6443-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PH-3

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
3-Penten-2-one, 4...	4.42	3.9	ng	120336	1	6.85	623420	20.0
2-Pentanone, 4-hy...	5.05	15.7	ng	490679	1	6.85	623420	20.0
unknown6.62	6.62	74.2	ng	2313710	1	6.85	623420	20.0
n-Hexadecanoic acid	11.92	8.4	ng	397536	4	11.39	947156	20.0
Pyrene, 1-methyl-	13.17	2.1	ng	103961	5	14.04	986971	20.0
Cyclopentadecane	13.88	6.5	ng	319967	5	14.04	986971	20.0
Squalene	14.89	2.4	ng	122664	6	15.54	1035810	20.0
Benzo[e]pyrene	15.41	2.1	ng	109307	6	15.54	1035810	20.0