LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098806.D
Acq On : 26 Sep 2017 2:17
Operator : SJ/JU
Sample : I5362-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2-B-COMP

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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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	2.198	15	19	26	rVB	53220	75740	2.00%	0.185%
2	5.139	515	519	532	rVB	500934	650267	17.14%	1.586%
3	5.533	578	586	589	rBV	3291131	3392432	89.41%	8.275%
4	6.539	751	757	760	rBV	3185694	3500593	92.26%	8.539%
5	6.686	777	782	785	rBV	3539986	3513607	92.60%	8.571%
6	6.745	788	792	795	rBV	46247	44834	1.18%	0.109%
7	6.916	817	821	824	rVB	1210920	976488	25.74%	2.382%
8	7.074	843	848	851	rBV	2808492	2667485	70.30%	6.507%
9	7.474	911	916	919	rBV	2133754	2221034	58.54%	5.418%
10	7.545	925	928	934	rVB2	45014	49157	1.30%	0.120%
11	8.198	1035	1039	1041	rBV	1543113	1320646	34.81%	3.221%
12	8.215	1041	1042	1045	rVB	141464	87440	2.30%	0.213%
13	8.468	1082	1085	1090	rBV3	37861	40412	1.07%	0.099%
14	8.904	1156	1159	1162	rVB	86734	69457	1.83%	0.169%
15	9.004	1173	1176	1180	rBV	68720	58990	1.55%	0.144%
16	9.268	1216	1221	1225	rBV	3842708	3794240	100.00%	9.255%
17	9.345	1231	1234	1236	rBV2	54547	48070	1.27%	0.117%
18	9.527	1262	1265	1269	rVB2	38582	47552	1.25%	0.116%
19	9.604	1276	1278	1281	rBV	62850	64959	1.71%	0.158%
20	9.662	1285	1288	1291	rVB	582202	496596	13.09%	1.211%
21	9.809	1310	1313	1316	rBV	99377	80792	2.13%	0.197%
22	9.874	1319	1324	1326	rVB	78912	67511	1.78%	0.165%
23	9.951	1328	1337	1340	rBV2	1683402	1469934	38.74%	3.586%
24	9.980	1340	1342	1345	rVB	83223	71143	1.88%	0.174%
25	10.151	1365	1371	1375	rVB	101691	110921	2.92%	0.271%
26	10.192	1375	1378	1382	rVB3	48484	44378	1.17%	0.108%
27	10.262	1387	1390	1392	rBV3	47359	48119	1.27%	0.117%
28	10.356	1402	1406	1407	rBV3	52855	65240	1.72%	0.159%
29	10.374	1407	1409	1412	rVB	143415	104008	2.74%	0.254%
30	10.498	1426	1430	1435	rVB2	79557	92203	2.43%	0.225%
31	10.592	1442	1446	1448	rBV	45144	60411	1.59%	0.147%
32	10.651	1452	1456	1459	rBV3	41675	46654	1.23%	0.114%
33	10.739	1467	1471	1474	rVB	2099486	1955128	51.53%	4.769%
34	10.845	1486	1489	1495	rBV	179451	251070	6.62%	0.612%

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Sample : I5362-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2-B-COMP

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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.933	1502	1504	1508	rBV4	26457	39630	1.04%	0.097%
36	11.039	1518	1522	1525	rBV4	45130	66655	1.76%	0.163%
37	11.168	1540	1544	1546	rBV4	49075	58287	1.54%	0.142%
38	11.192	1546	1548	1553	rVV5	47786	69099	1.82%	0.169%
39	11.239	1553	1556	1559	rVV2	57874	62657	1.65%	0.153%
40	11.292	1561	1565	1568	rVV2	156224	166493	4.39%	0.406%
41	11.327	1568	1571	1577	rVB3	64935	100809	2.66%	0.246%
42	11.439	1586	1590	1592	rBV	1487797	1282651	33.81%	3.129%
43	11.462	1592	1594	1597	rVV	485265	387438	10.21%	0.945%
44	11.509	1600	1602	1605	rVB	167649	132022	3.48%	0.322%
45	11.662	1626	1628	1634	rBV3	30375	43648	1.15%	0.106%
46	11.721	1635	1638	1642	rVB2	87214	83763	2.21%	0.204%
47	11.956	1672	1678	1685	rBV2	217028	392086	10.33%	0.956%
48	12.015	1685	1688	1690	rBV	56380	58425	1.54%	0.143%
49	12.050	1690	1694	1696	rBV2	147609	161419	4.25%	0.394%
50	12.127	1704	1707	1712	rBV2	99979	116097	3.06%	0.283%
51	12.233	1722	1725	1727	rBV	86231	67789	1.79%	0.165%
52	12.380	1748	1750	1753	rVB2	58814	50617	1.33%	0.123%
53	12.415	1753	1756	1758	rBV2	39754	39844	1.05%	0.097%
54	12.486	1766	1768	1771	rBV	86341	82271	2.17%	0.201%
55	12.515	1771	1773	1777	rVV3	98023	103583	2.73%	0.253%
56	12.574	1781	1783	1788	rBV3	56843	70229	1.85%	0.171%
57	12.650	1793	1796	1800	rBV	891714	726300	19.14%	1.772%
58	12.745	1809	1812	1815	rBV	53491	59551	1.57%	0.145%
59	12.833	1824	1827	1830	rBV	243758	183280	4.83%	0.447%
60	12.880	1830	1835	1842	rBV	812769	858003	22.61%	2.093%
61	13.021	1855	1859	1866	rVB	2769879	2578364	67.95%	6.289%
62	13.097	1868	1872	1876	rBV4	68718	119414	3.15%	0.291%
63	13.180	1884	1886	1888	rBV3	43009	46864	1.24%	0.114%
64	13.203	1888	1890	1894	rVB	124398	123028	3.24%	0.300%
65	13.245	1894	1897	1899	rBV	87795	80684	2.13%	0.197%
66	13.274	1899	1902	1905	rVV	93028	73688	1.94%	0.180%
67	13.309	1905	1908	1911	rVV2	91005	92711	2.44%	0.226%
68	13.403	1922	1924	1926	rVB	53994	39391	1.04%	0.096%
69	13.433	1927	1929	1932	rVB	61713	51386	1.35%	0.125%
70	13.539	1945	1947	1950	rVB	138390	95661	2.52%	0.233%
71	13.586	1952	1955	1957	rBV	93123	86764	2.29%	0.212%

LSC Area Percent Report

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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2-B-COMP

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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	13.709	1974	1976	1981	rVB	74401	84956	2.24%	0.207%
73	13.903	2006	2009	2016	rVB4	411624	452721	11.93%	1.104%
74	14.074	2034	2038	2041	rBV2	987373	1234606	32.54%	3.012%
75	14.103	2041	2043	2049	rVB	365294	332477	8.76%	0.811%
76	14.539	2114	2117	2122	rVB3	146965	193740	5.11%	0.473%
77	15.127	2213	2217	2220	rBV	323481	485374	12.79%	1.184%
78	15.191	2226	2228	2231	rBV2	97100	103521	2.73%	0.253%
79	15.438	2267	2270	2277	rVB	222878	276924	7.30%	0.676%
80	15.503	2277	2281	2287	rBV	293007	373213	9.84%	0.910%
81	15.574	2288	2293	2304	rVB2	625975	1019341	26.87%	2.487%

Sum of corrected areas: 40994985

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098806.D
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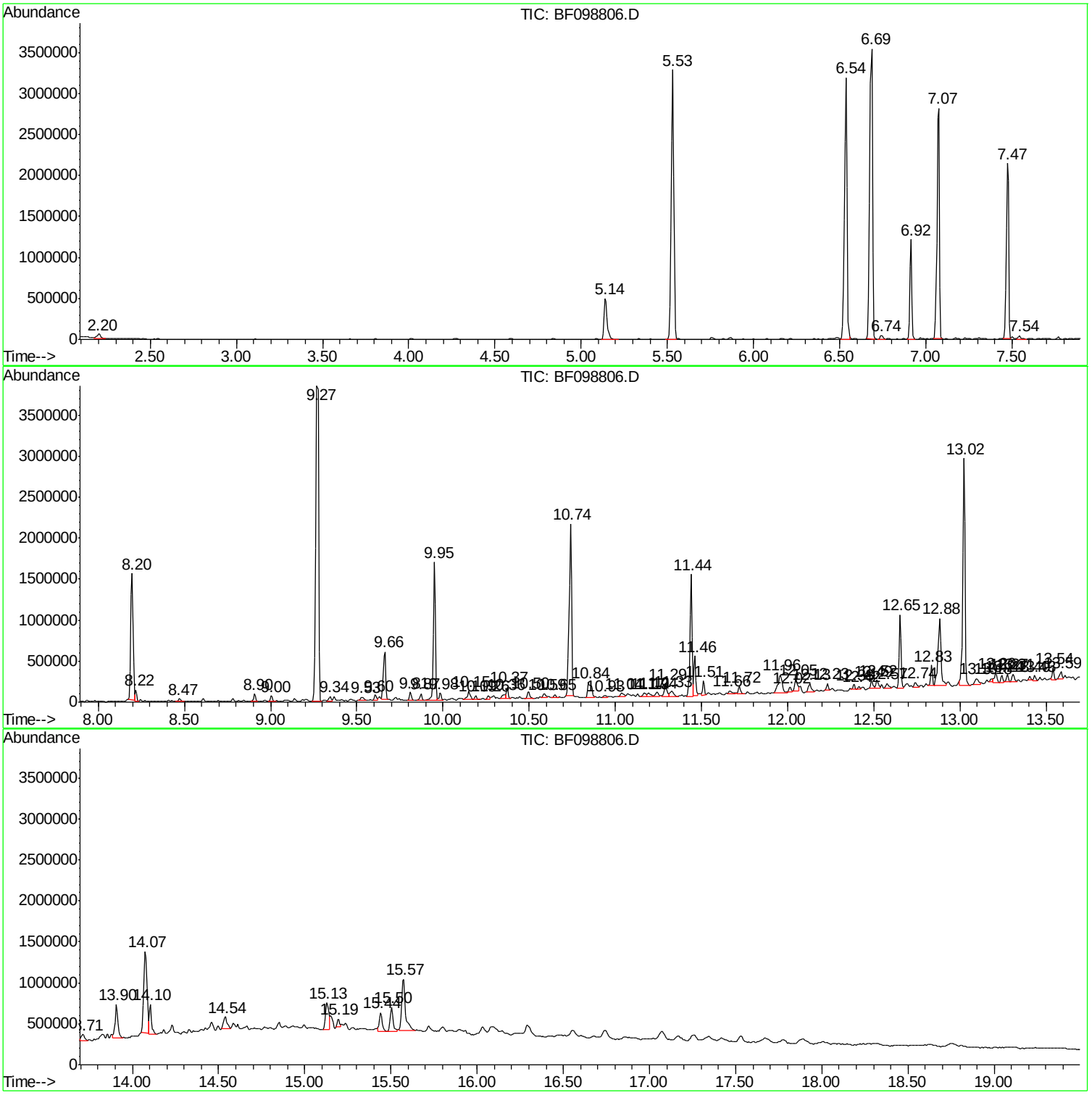
Operator : SJ/JU
Sample : I5362-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098806.D
Acq On : 26 Sep 2017 2:17
Operator : SJ/JU
Sample : I5362-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

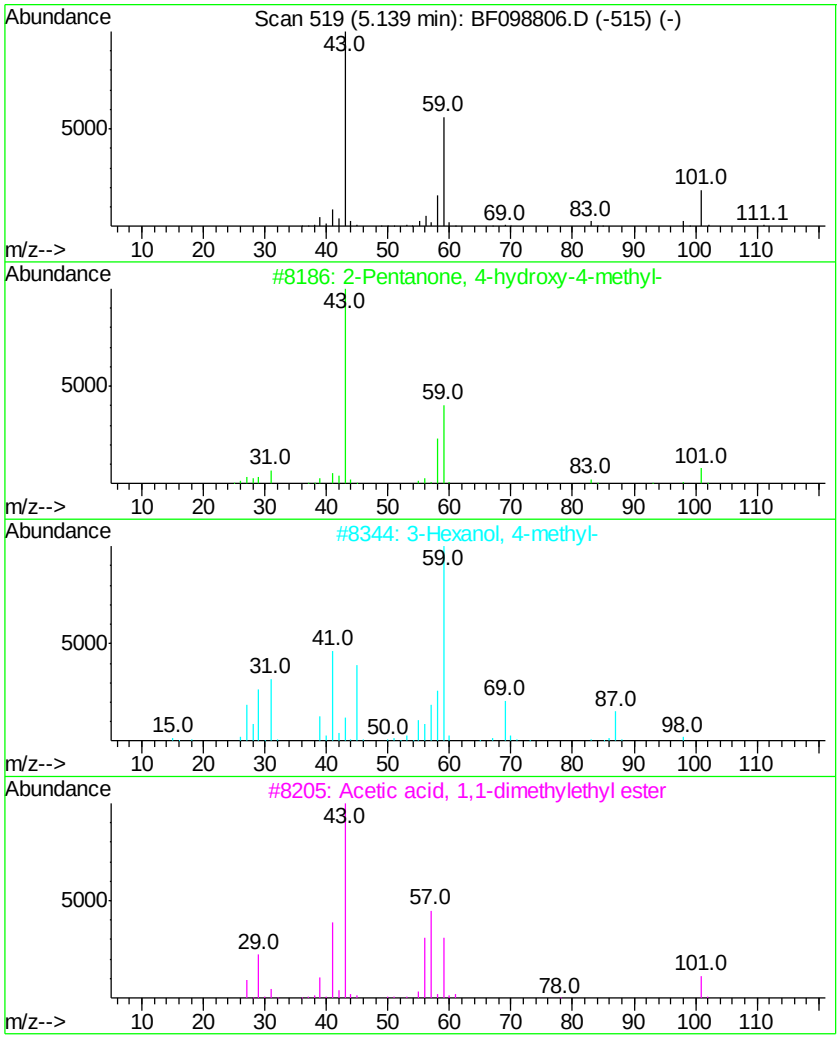
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

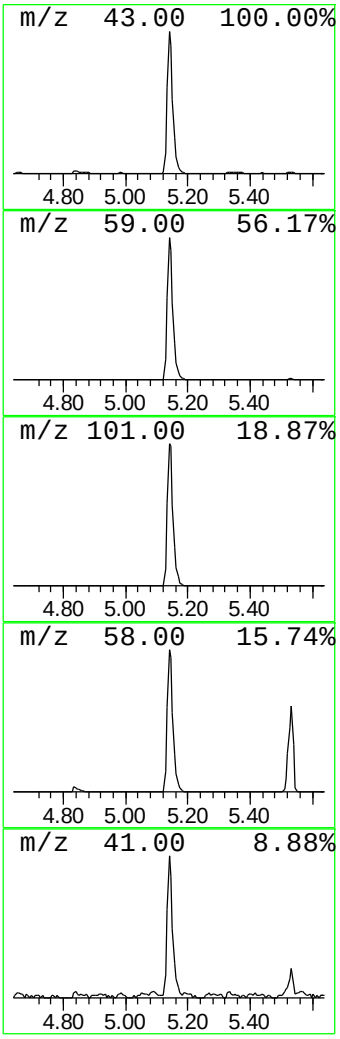
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	13.32 ng	650267	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23





Library Search Compound Report

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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

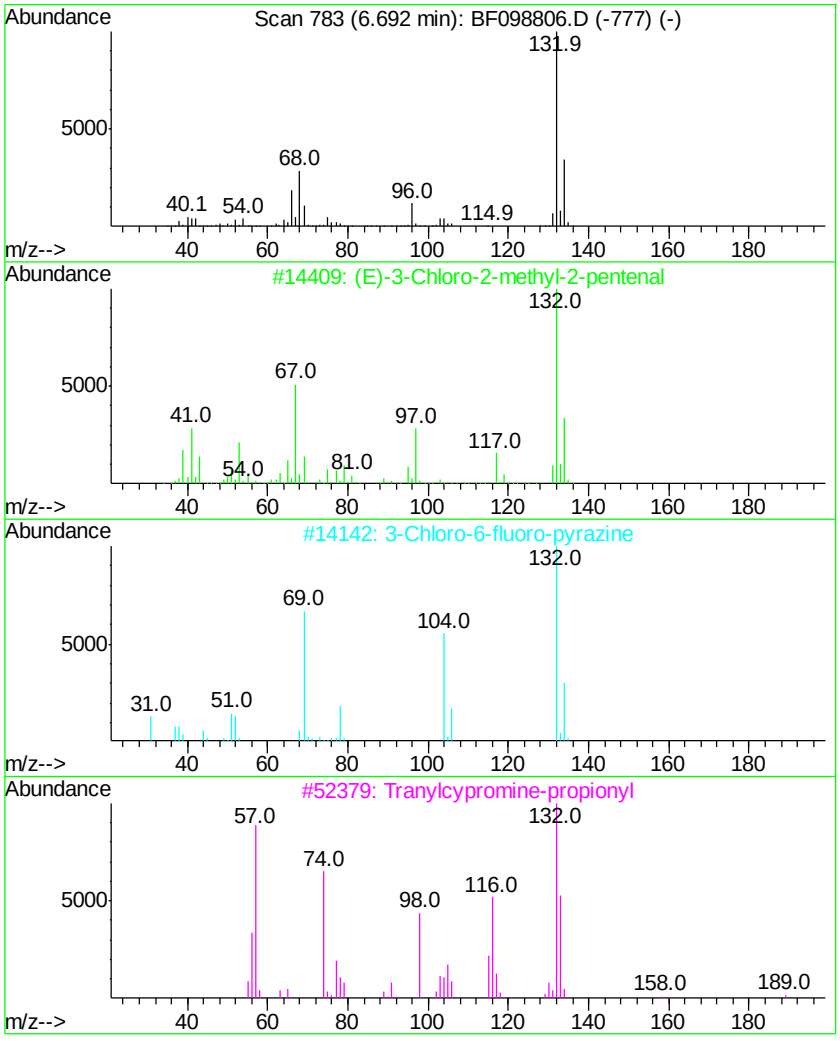
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

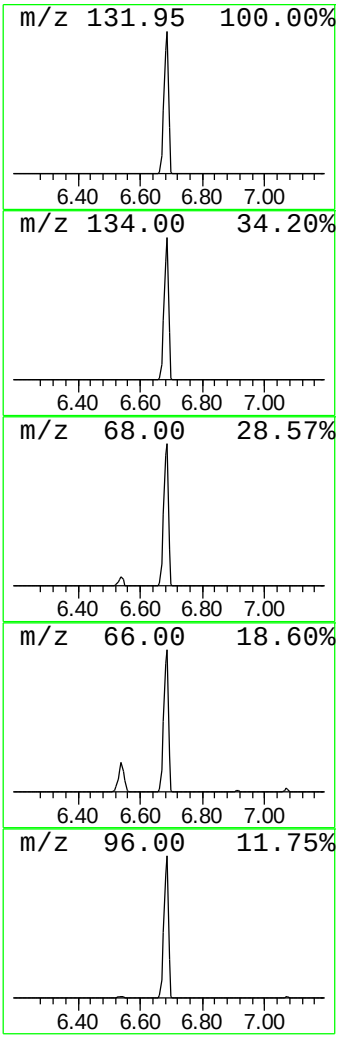
****

Peak Number 2 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	71.96 ng	3513610	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Library : C:\DATABASE\NIST11.L
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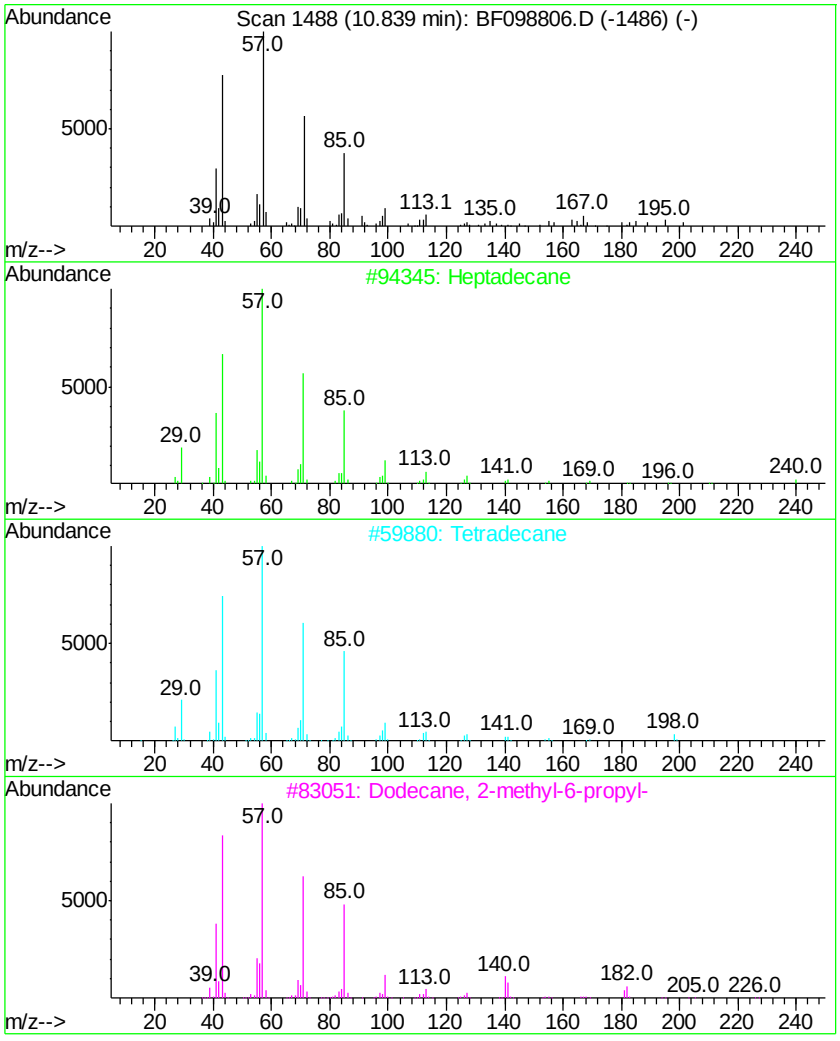
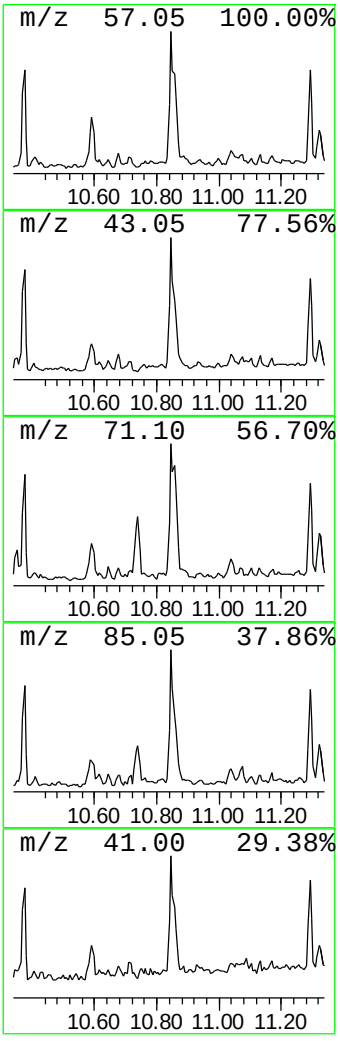
****

Peak Number 4 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	3.91 ng	251070	Phenanthrene-d10	11.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Tetradecane	198	C14H30	000629-59-4	87
3	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80
4	Pentadecane	212	C15H32	000629-62-9	64
5	Hexadecane	226	C16H34	000544-76-3	64





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TIC Library : C:\DATABASE\NIST11.L
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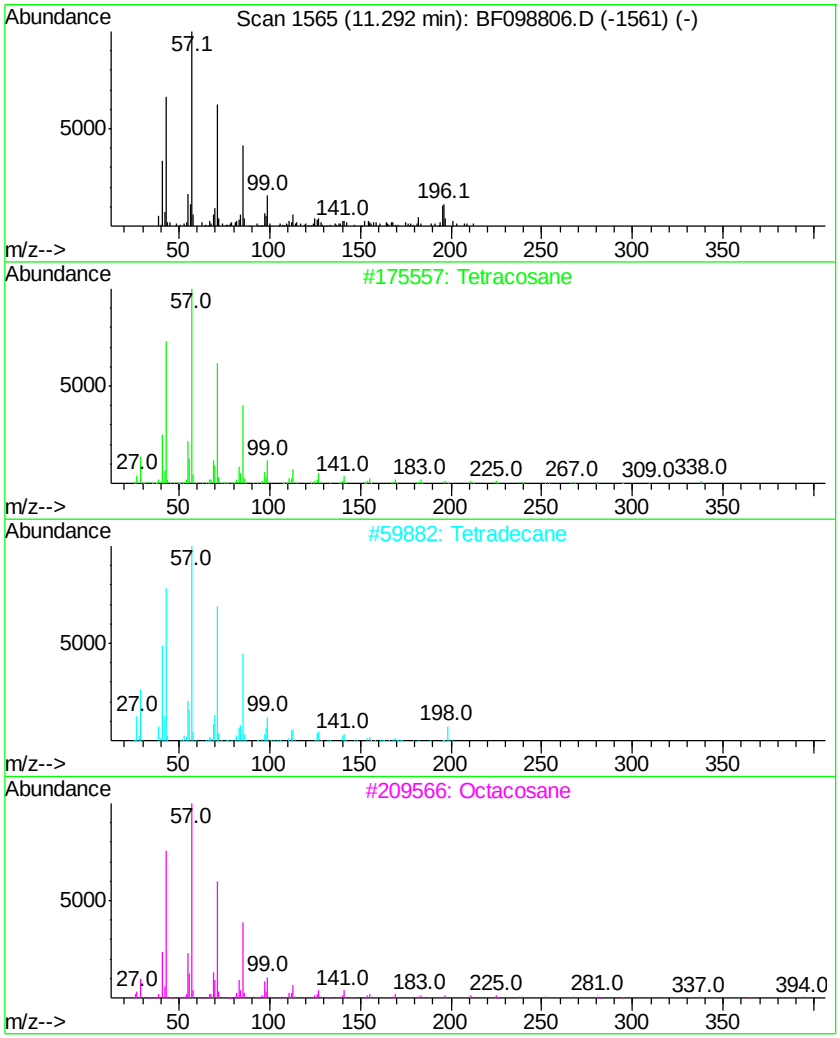
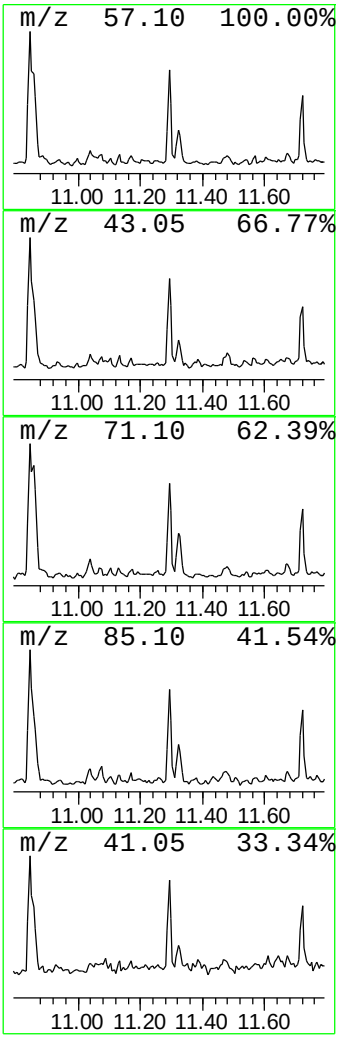
****

Peak Number 5 Tetracosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.29	2.60 ng	166493	Phenanthrene-d10	11.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	68
2	Tetradecane	198	C14H30	000629-59-4	68
3	Octacosane	394	C28H58	000630-02-4	68
4	Heptacosane	380	C27H56	000593-49-7	64
5	Hexadecane	226	C16H34	000544-76-3	64





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Sample : I5362-03
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ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

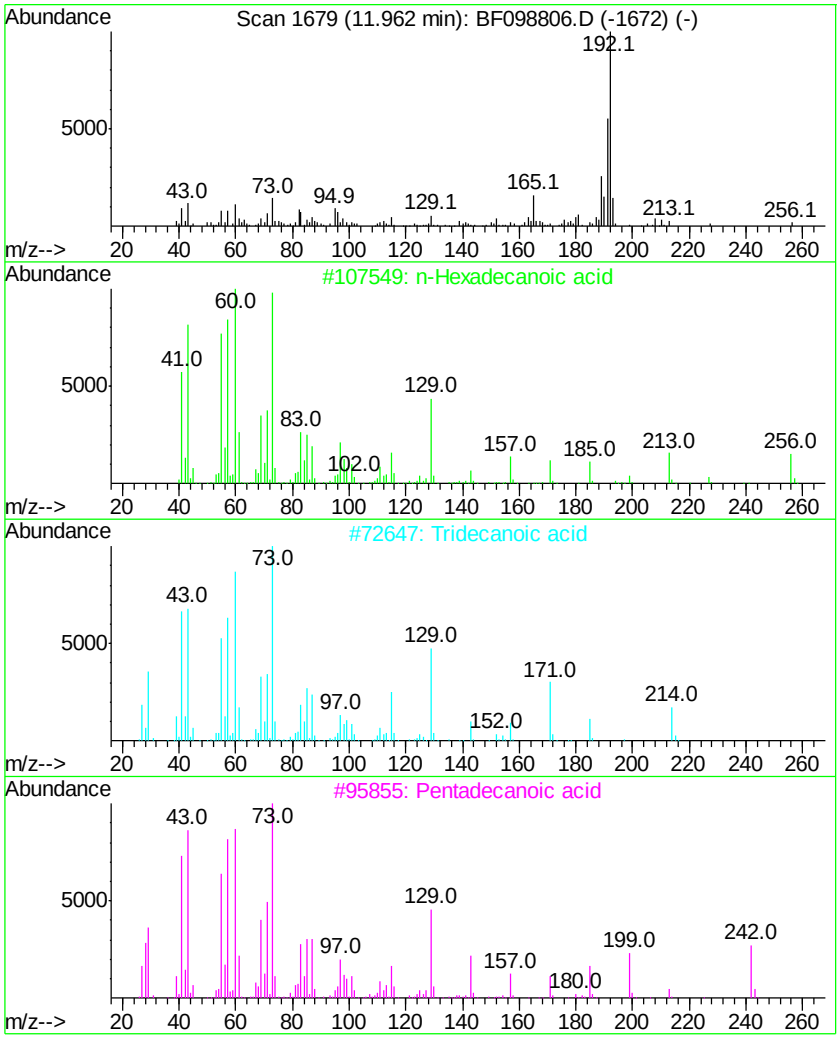
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

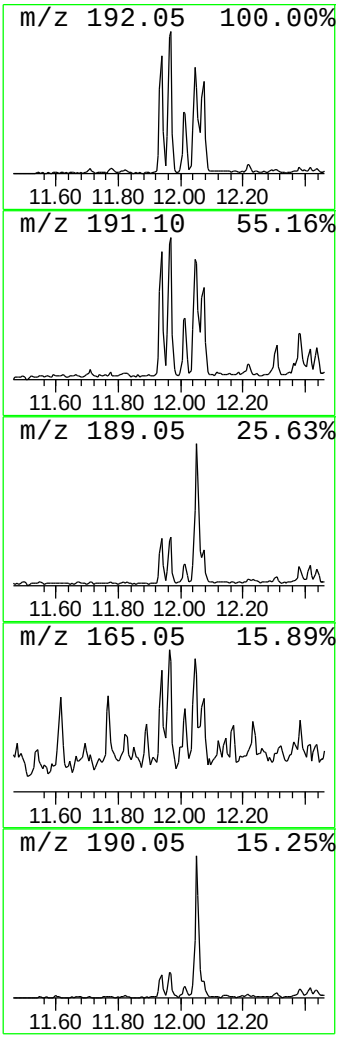
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	6.11 ng	392086	Phenanthrene-d10	11.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Undecanoic acid	186	C11H22O2	000112-37-8	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53





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Operator : SJ/JU
Sample : I5362-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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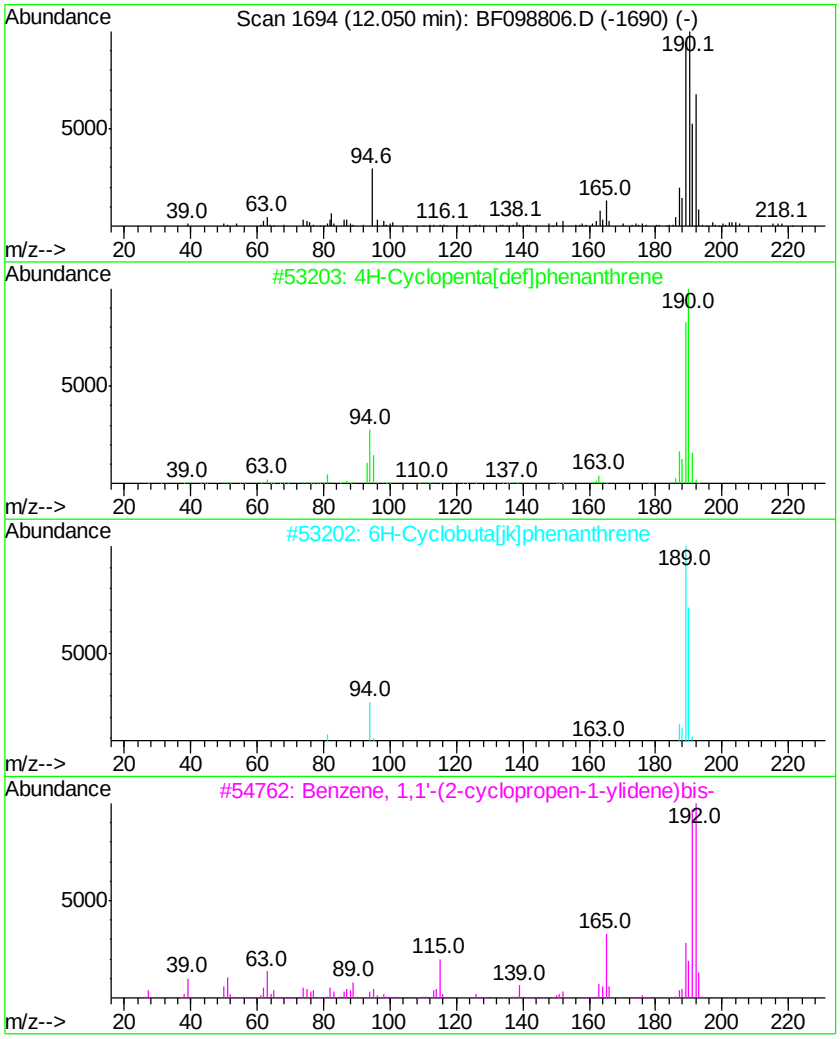
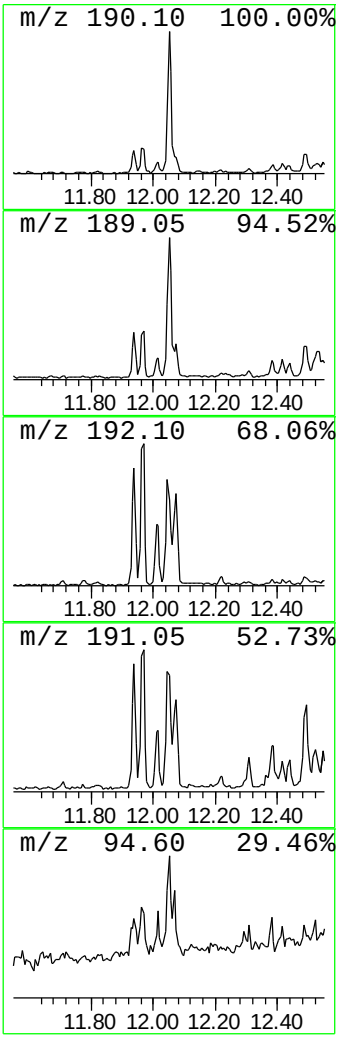
Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	2.52 ng	161419	Phenanthrene-d10	11.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	40
3	Benzene, 1,1'-(2-cyclopropen-1-y...	192	C15H12	022825-21-4	22
4	8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	20
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	18





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098806.D
Acq On : 26 Sep 2017 2:17
Operator : SJ/JU
Sample : I5362-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

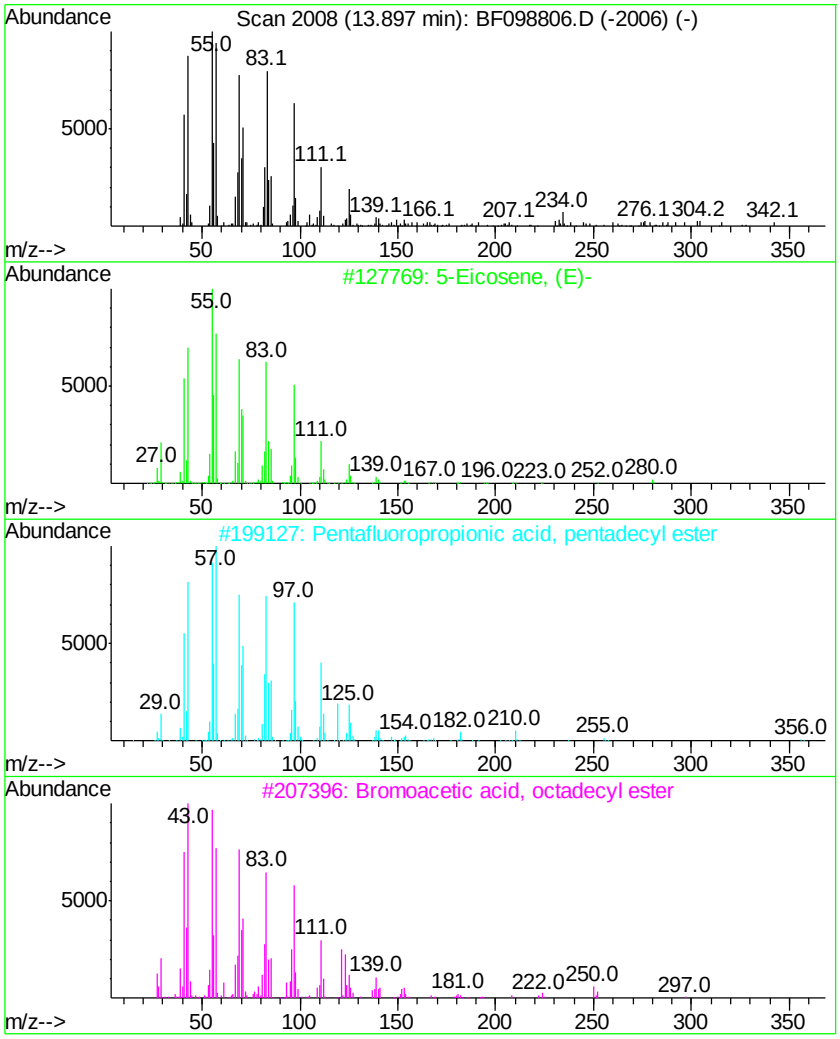
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

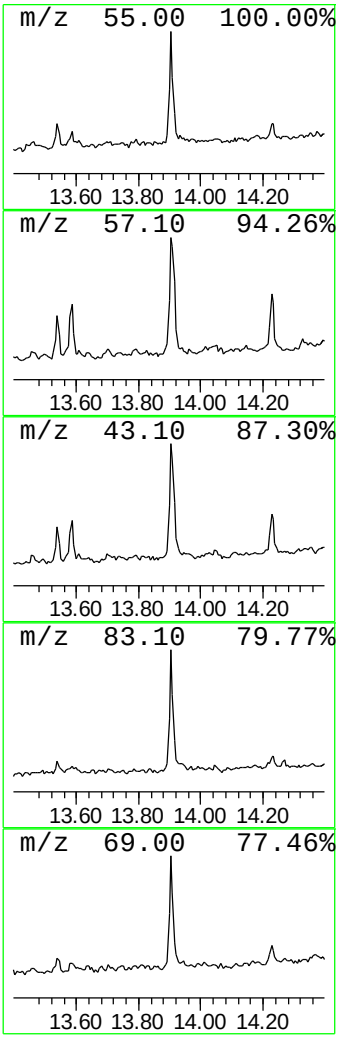
****

Peak Number 8 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	7.33 ng	452721	Chrysene-d12	14.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	95
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
3	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092517\
Data File : BF098806.D
Acq On : 26 Sep 2017 2:17
Operator : SJ/JU
Sample : I5362-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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...	5.14	13.3	ng	650267	1	6.92	976488	20.0
unknown6.69	6.69	72.0	ng	3513610	1	6.92	976488	20.0
Heptadecane	10.84	3.9	ng	251070	4	11.44	1282650	20.0
Tetracosane	11.29	2.6	ng	166493	4	11.44	1282650	20.0
n-Hexadecanoic acid	11.96	6.1	ng	392086	4	11.44	1282650	20.0
4H-Cyclopenta[def...	12.05	2.5	ng	161419	4	11.44	1282650	20.0
5-Eicosene, (E)-	13.90	7.3	ng	452721	5	14.08	1234610	20.0