LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102898.D
Acq On : 9 Feb 2018 19:32
Operator : SJ/JU
Sample : J1512-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-2334

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-BF020318.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	2.169	7	14	23	rVB	453295	621852	14.77%	1.562%
2	5.116	512	515	525	rVB	108902	147599	3.51%	0.371%
3	5.504	576	581	585	rBV	3929228	4210588	100.00%	10.573%
4	6.516	747	753	764	rBV	3681789	4210510	100.00%	10.573%
5	6.657	772	777	780	rBV	4191139	4018762	95.44%	10.092%
6	6.886	812	816	819	rBV	1288878	1119120	26.58%	2.810%
7	7.039	838	842	846	rBV	3307851	3086622	73.31%	7.751%
8	7.445	906	911	914	rBV	2692800	2680515	63.66%	6.731%
9	7.522	921	924	932	rVB	34977	42866	1.02%	0.108%
10	7.622	938	941	944	rVB	55566	49203	1.17%	0.124%
11	8.169	1030	1034	1037	rBV	1627214	1421455	33.76%	3.569%
12	9.239	1212	1216	1220	rBV	3699452	3544291	84.18%	8.900%
13	9.316	1226	1229	1231	rVB	63075	49126	1.17%	0.123%
14	9.633	1279	1283	1286	rBV	437393	395750	9.40%	0.994%
15	9.786	1306	1309	1311	rBV	62631	56569	1.34%	0.142%
16	9.845	1311	1319	1323	rVV	201742	162260	3.85%	0.407%
17	9.922	1328	1332	1336	rBV2	1454890	1321101	31.38%	3.317%
18	10.163	1371	1373	1378	rBV2	39884	43105	1.02%	0.108%
19	10.345	1401	1404	1407	rVB	239537	175326	4.16%	0.440%
20	10.563	1434	1441	1444	rBV	53915	74717	1.77%	0.188%
21	10.710	1463	1466	1477	rVV	1834573	1878605	44.62%	4.717%
22	10.816	1481	1484	1494	rVB	162111	196846	4.68%	0.494%
23	11.269	1558	1561	1563	rBV	71714	59024	1.40%	0.148%
24	11.410	1581	1585	1588	rBV	1207666	1113762	26.45%	2.797%
25	11.433	1588	1589	1595	rVB	191941	139292	3.31%	0.350%
26	11.916	1667	1671	1672	rBV	38233	43276	1.03%	0.109%
27	11.939	1672	1675	1681	rVB2	54951	73651	1.75%	0.185%
28	12.021	1686	1689	1692	rBV2	49085	57322	1.36%	0.144%
29	12.463	1757	1764	1767	rBV3	38178	56641	1.35%	0.142%
30	12.621	1788	1791	1795	rBV	367705	349221	8.29%	0.877%
31	12.857	1825	1831	1834	rBV	334099	380813	9.04%	0.956%
32	12.998	1847	1855	1858	rBV	2603505	2565750	60.94%	6.443%
33	13.063	1863	1866	1872	rBV3	54253	79541	1.89%	0.200%
34	13.157	1879	1882	1884	rBV4	37975	46073	1.09%	0.116%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102898.D
Acq On : 9 Feb 2018 19:32
Operator : SJ/JU
Sample : J1512-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-2334

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-BF020318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.180	1884	1886	1890	rVV2	55173	52406	1.24%	0.132%
36	13.215	1890	1892	1895	rVV	55611	48595	1.15%	0.122%
37	13.286	1900	1904	1907	rVV2	51816	52905	1.26%	0.133%
38	13.527	1941	1945	1947	rBV	41506	42161	1.00%	0.106%
39	13.686	1970	1972	1977	rVB	52515	55314	1.31%	0.139%
40	13.798	1985	1991	1994	rBV2	54815	84218	2.00%	0.211%
41	13.880	2002	2005	2011	rVB4	320850	388012	9.22%	0.974%
42	14.021	2026	2029	2030	rBV	198677	155255	3.69%	0.390%
43	14.051	2030	2034	2037	rVV2	1287050	1374818	32.65%	3.452%
44	14.074	2037	2038	2045	rVB	242531	208946	4.96%	0.525%
45	14.198	2056	2059	2065	rVV5	34337	53233	1.26%	0.134%
46	14.439	2097	2100	2103	rVB	55081	50158	1.19%	0.126%
47	14.509	2109	2112	2119	rBV4	132585	198065	4.70%	0.497%
48	14.892	2175	2177	2181	rBV	44746	48287	1.15%	0.121%
49	15.098	2208	2212	2216	rBV	226386	383883	9.12%	0.964%
50	15.162	2220	2223	2226	rVV2	64798	78347	1.86%	0.197%
51	15.209	2228	2231	2235	rVB	57734	67559	1.60%	0.170%
52	15.409	2261	2265	2271	rVB	134060	180461	4.29%	0.453%
53	15.474	2271	2276	2281	rVB	175602	233612	5.55%	0.587%
54	15.539	2281	2287	2291	rBV	770463	1040727	24.72%	2.613%
55	15.756	2321	2324	2331	rVB8	35906	55489	1.32%	0.139%
56	15.992	2359	2364	2368	rBV3	50797	79888	1.90%	0.201%
57	16.051	2371	2374	2380	rVV8	32517	62066	1.47%	0.156%
58	16.115	2382	2385	2391	rVB6	27618	47838	1.14%	0.120%
59	17.039	2536	2542	2549	rVB3	67080	140278	3.33%	0.352%
60	17.492	2614	2619	2625	rVB2	46490	88900	2.11%	0.223%
61	17.727	2654	2659	2667	rVB9	38987	80206	1.90%	0.201%

Sum of corrected areas: 39822781

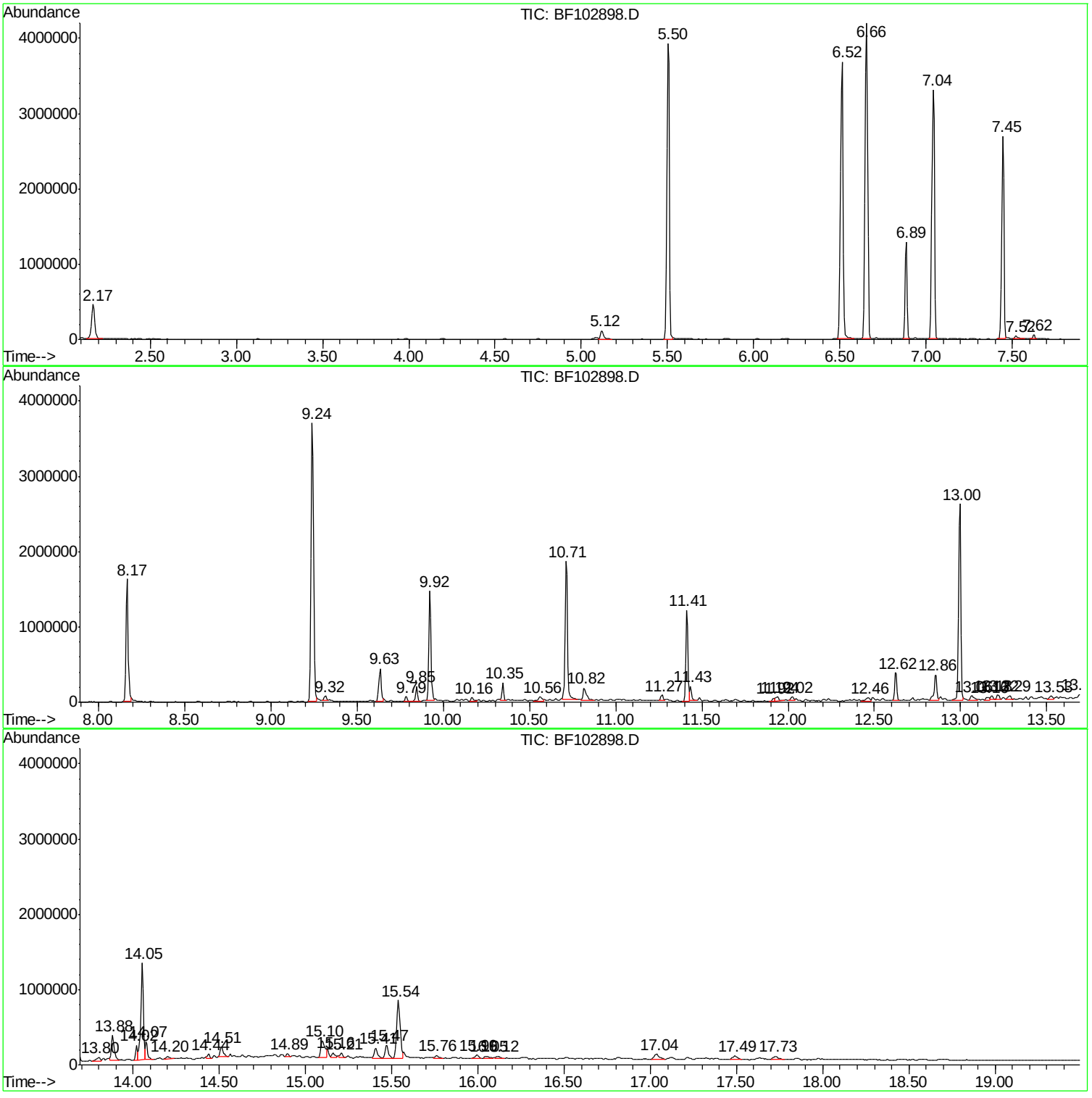
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102898.D
Acq On : 9 Feb 2018 19:32
Operator : SJ/JU
Sample : J1512-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-2334

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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\BF020918\
Data File : BF102898.D
Acq On : 9 Feb 2018 19:32
Operator : SJ/JU
Sample : J1512-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-2334

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

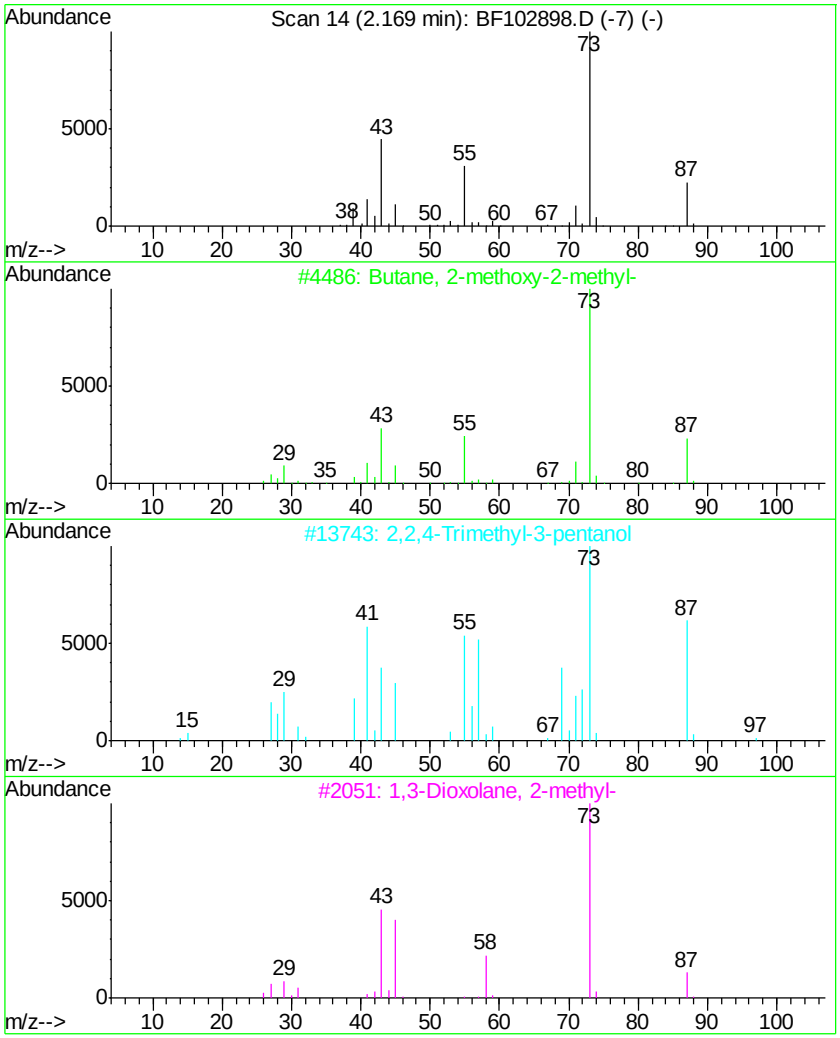
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

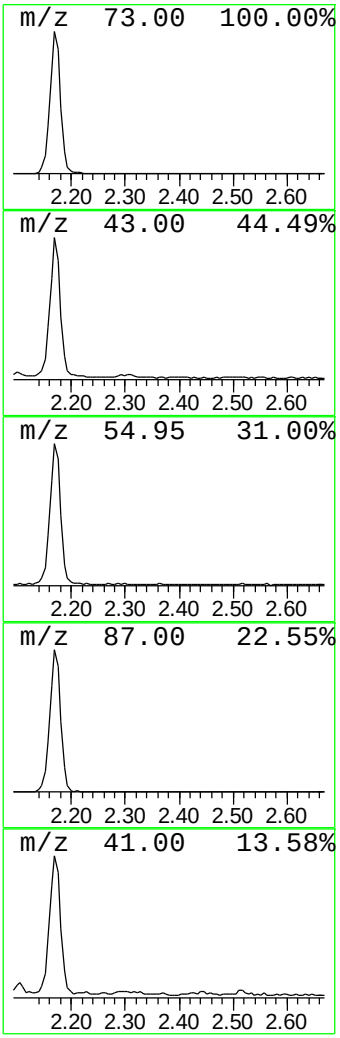
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	11.11 ng	621852	1,4-Dichlorobenzene-d4	6.89

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	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





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Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-2334

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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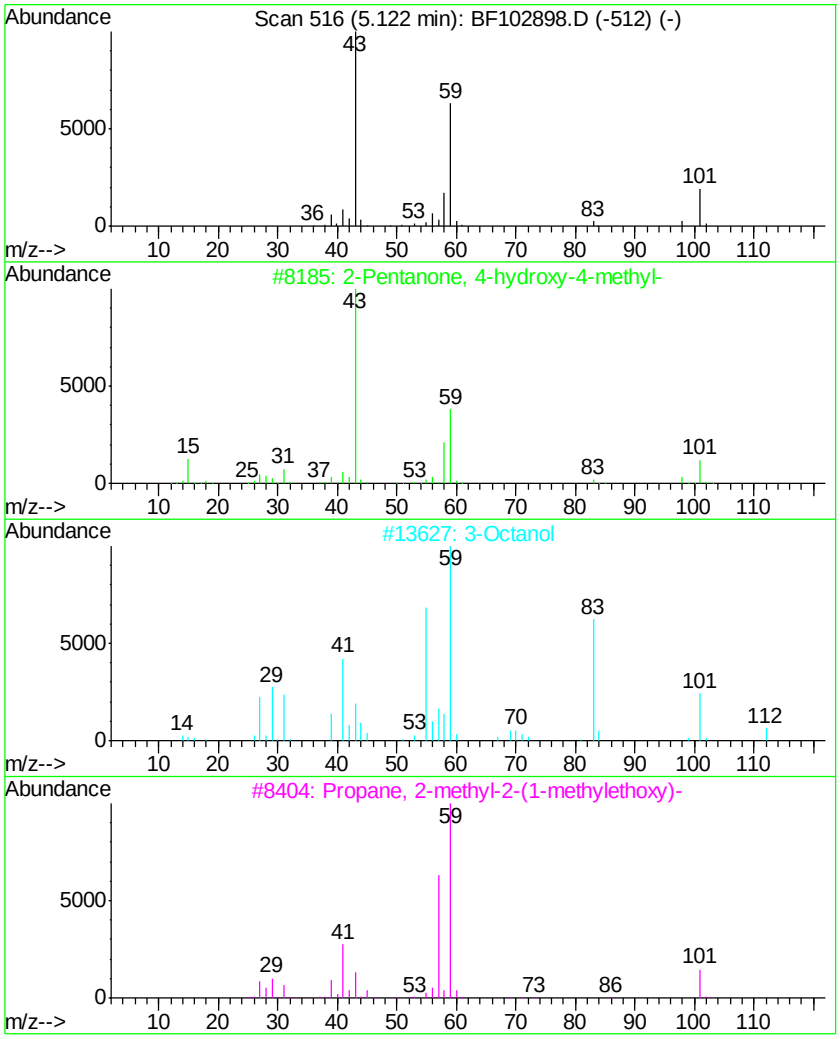
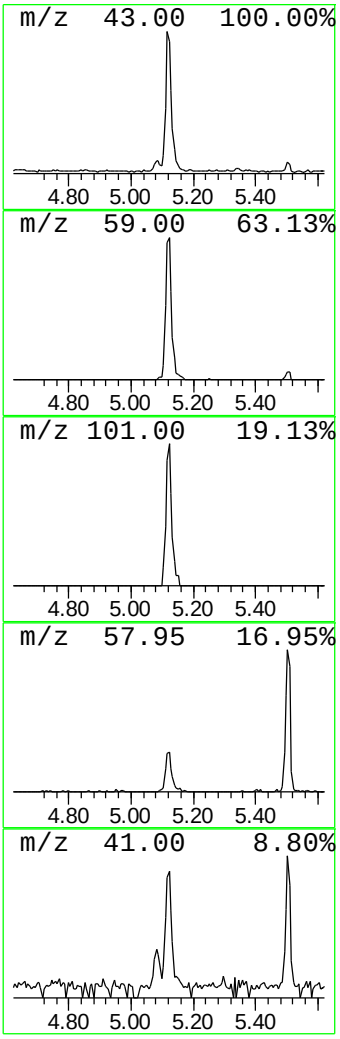
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	2.64 ng	147599	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Octanol	130	C8H18O	000589-98-0	36
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102898.D
Acq On : 9 Feb 2018 19:32
Operator : SJ/JU
Sample : J1512-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-2334

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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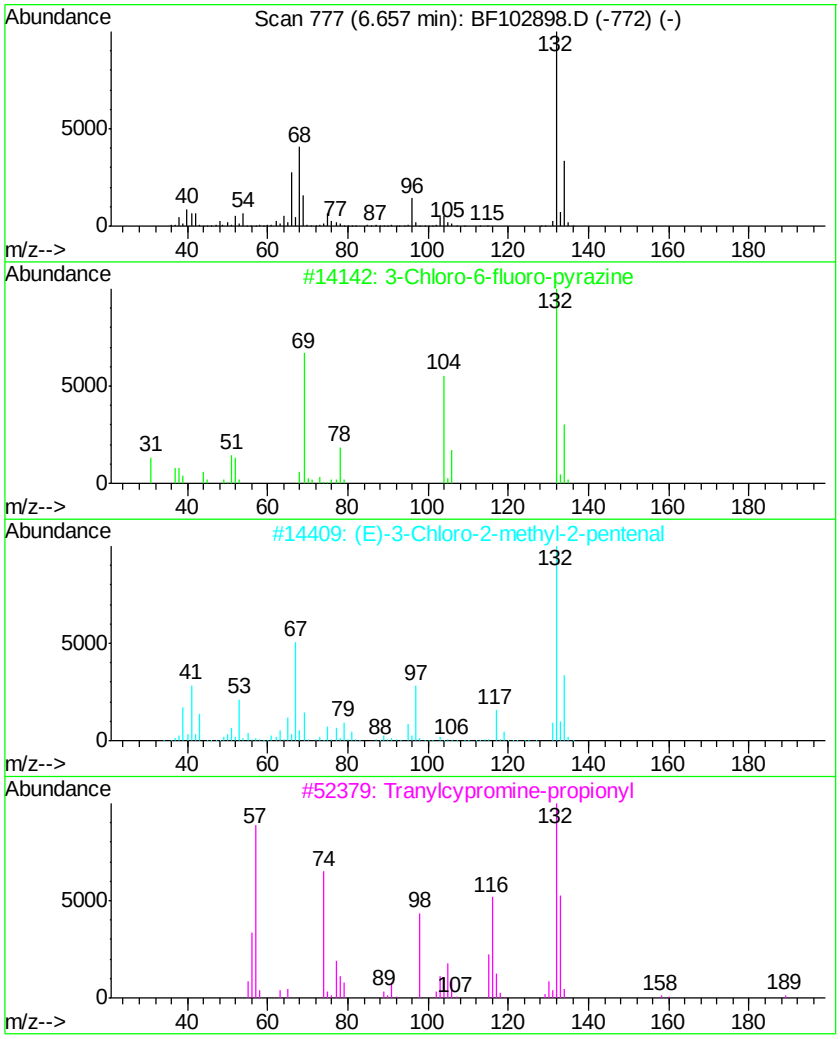
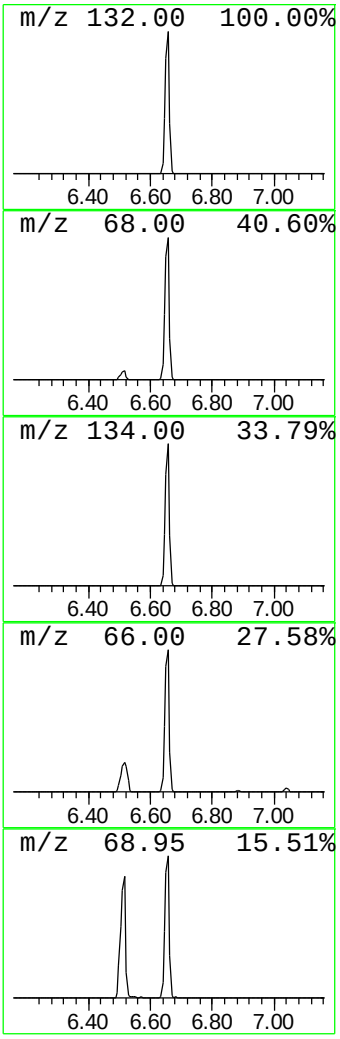
Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	71.82 ng	4018760	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102898.D
Acq On : 9 Feb 2018 19:32
Operator : SJ/JU
Sample : J1512-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-2334

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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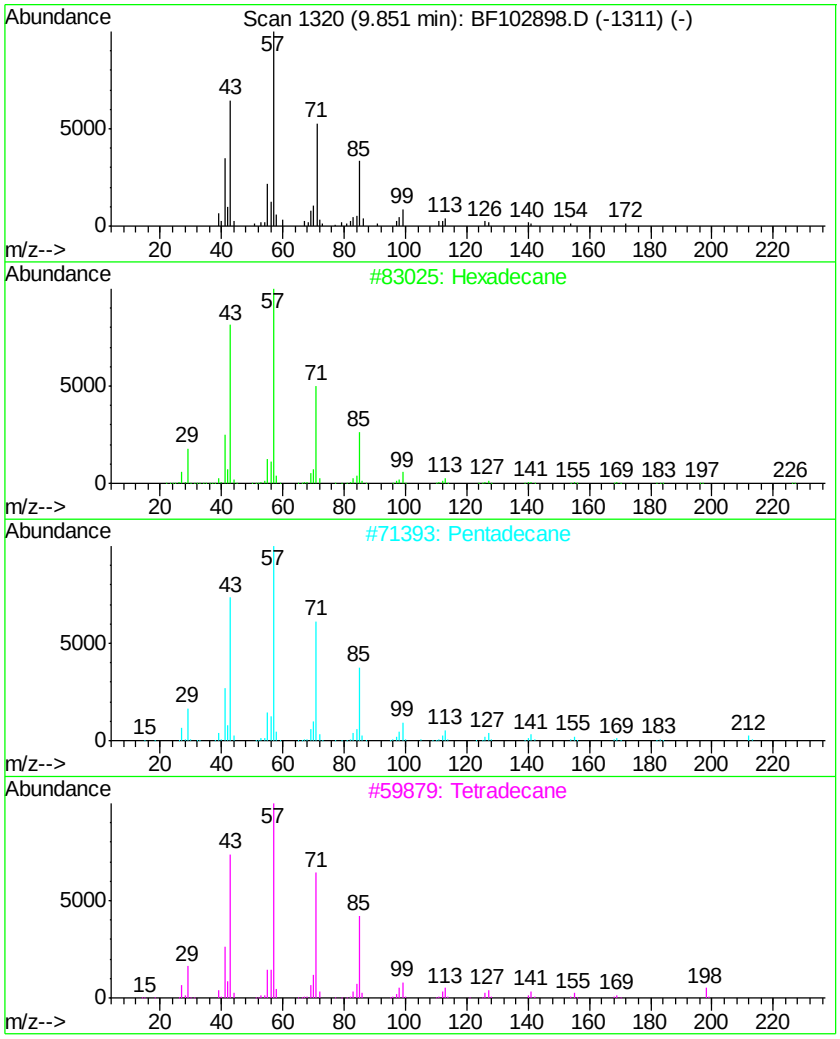
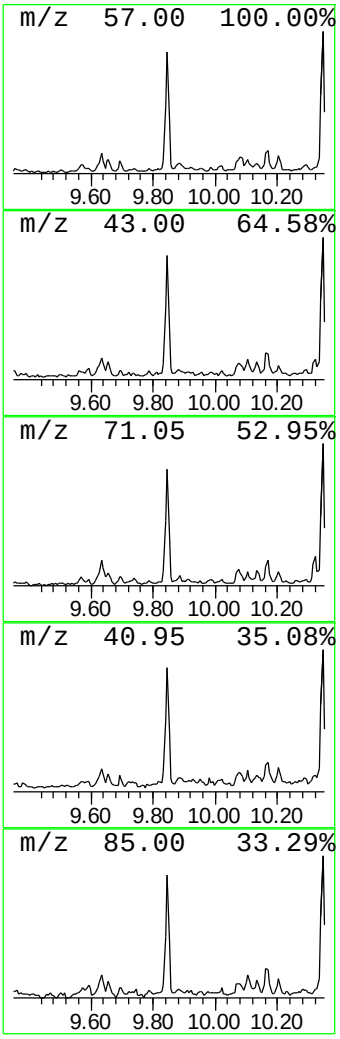
Peak Number 5 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.85	2.46 ng	162260	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	87
2	Pentadecane	212	C15H32	000629-62-9	80
3	Tetradecane	198	C14H30	000629-59-4	80
4	Tetradecane, 4-methyl-	212	C15H32	025117-24-2	72
5	Tridecane, 5-propyl-	226	C16H34	055045-11-9	72





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Misc :
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Instrument : BNA_F
ClientSampleId : RO-2334

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

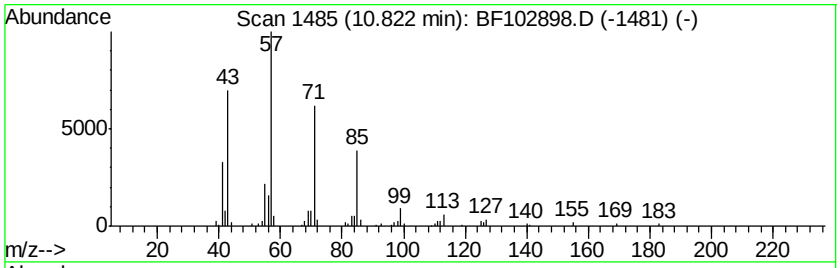
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

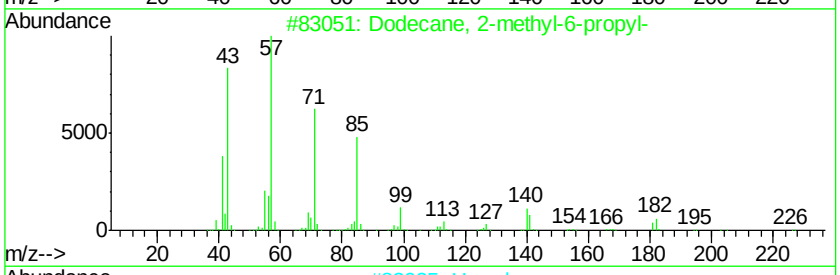
****

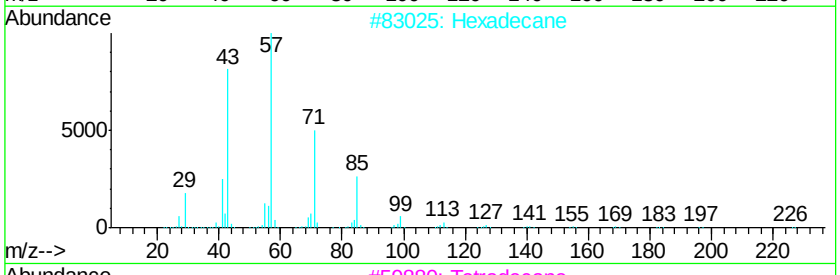
Peak Number 7 Dodecane, 2-methyl-6-propyl- Concentration Rank 5

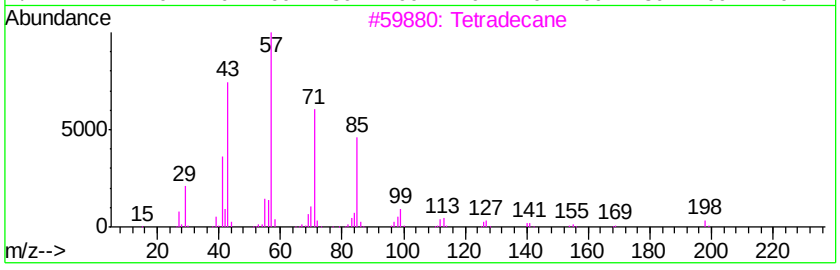
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	3.53 ng	196846	Phenanthrene-d10	11.41

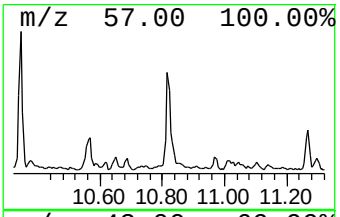
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86
2	Hexadecane	226	C16H34	000544-76-3	86
3	Tetradecane	198	C14H30	000629-59-4	80
4	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	72
5	Bacchotricuneatin c	342	C20H22O5	066563-30-2	64

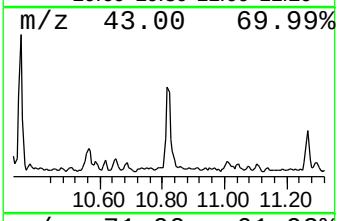


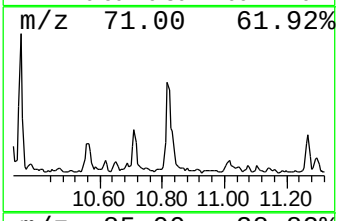


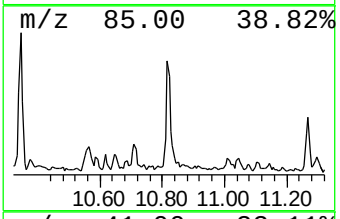


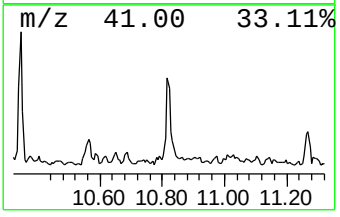












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Data File : BF102898.D
Acq On : 9 Feb 2018 19:32
Operator : SJ/JU
Sample : J1512-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-2334

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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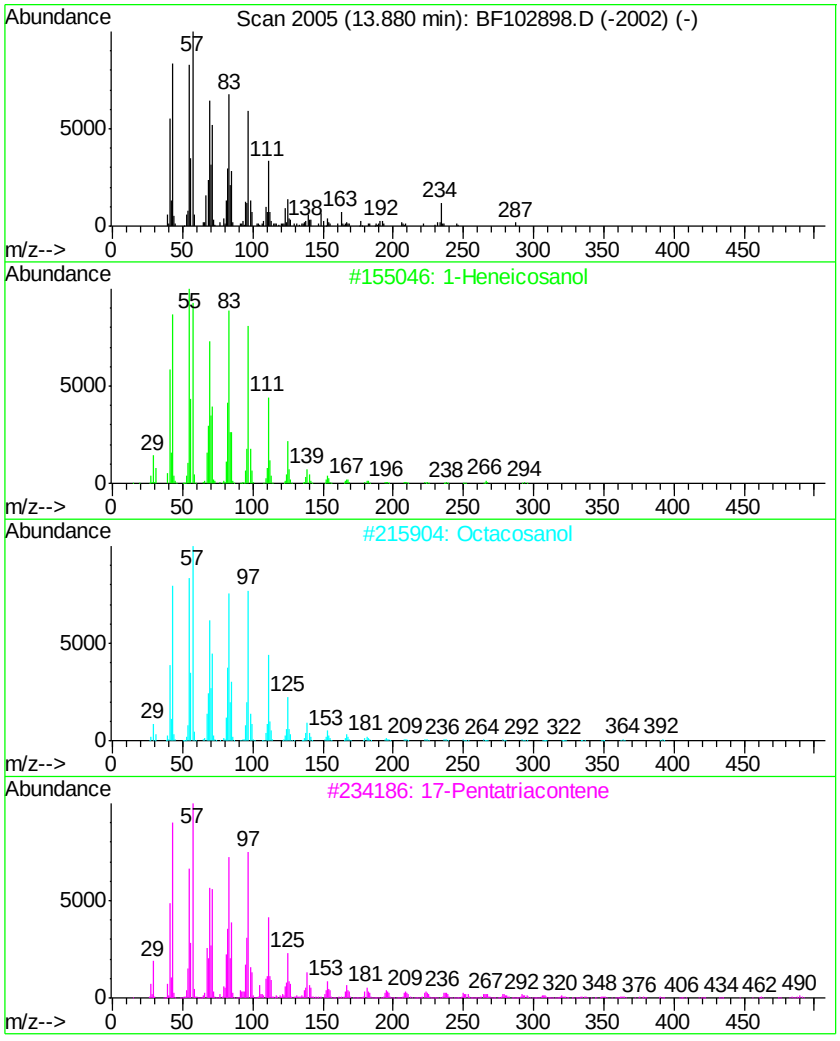
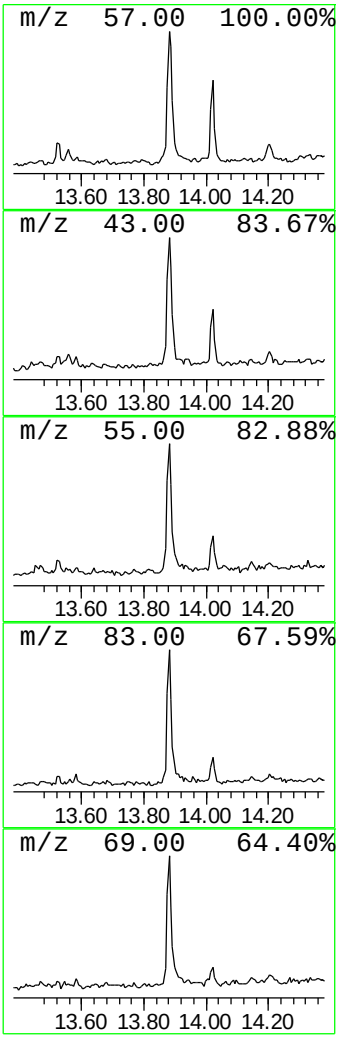
Peak Number 8 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	5.64 ng	388012	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	92
2	Octacosanol	410	C28H58O	000557-61-9	91
3	17-Pentatriacontene	491	C35H70	006971-40-0	90
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	87
5	1-Hexacosanol	382	C26H54O	000506-52-5	87





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Instrument : BNA_F
ClientSampleId : RO-2334

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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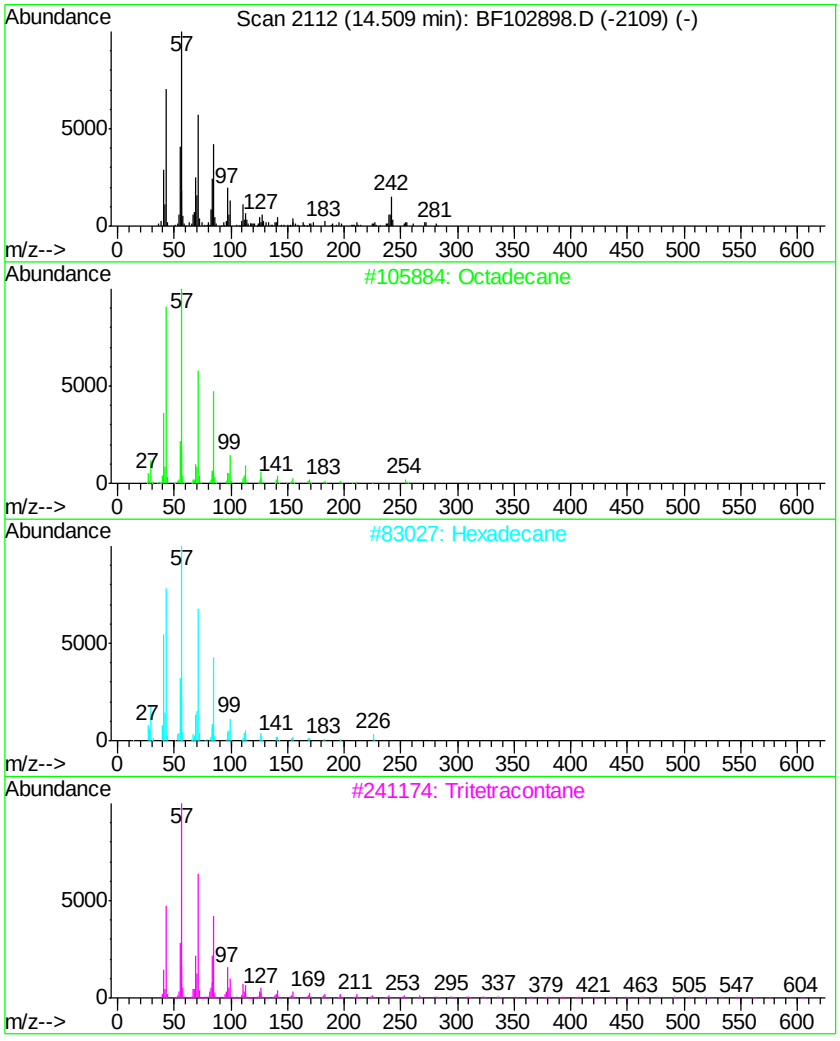
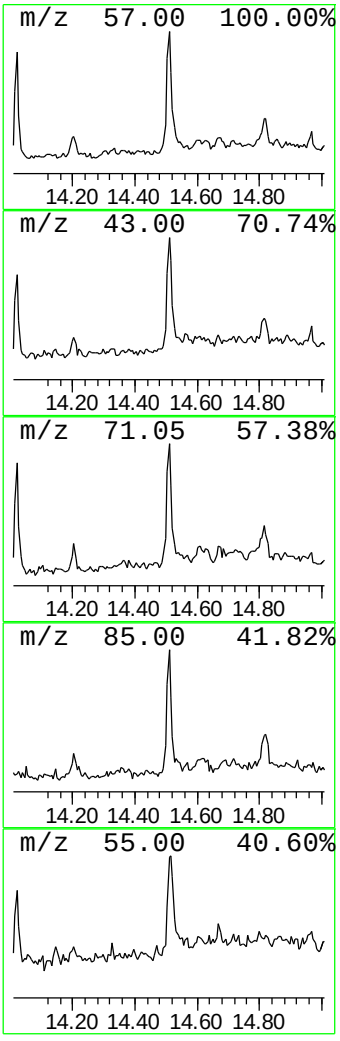
Peak Number 9 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.51	2.88 ng	198065	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	96
2	Hexadecane	226	C16H34	000544-76-3	96
3	Tritetracontane	605	C43H88	007098-21-7	90
4	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	90
5	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102898.D
Acq On : 9 Feb 2018 19:32
Operator : SJ/JU
Sample : J1512-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-2334

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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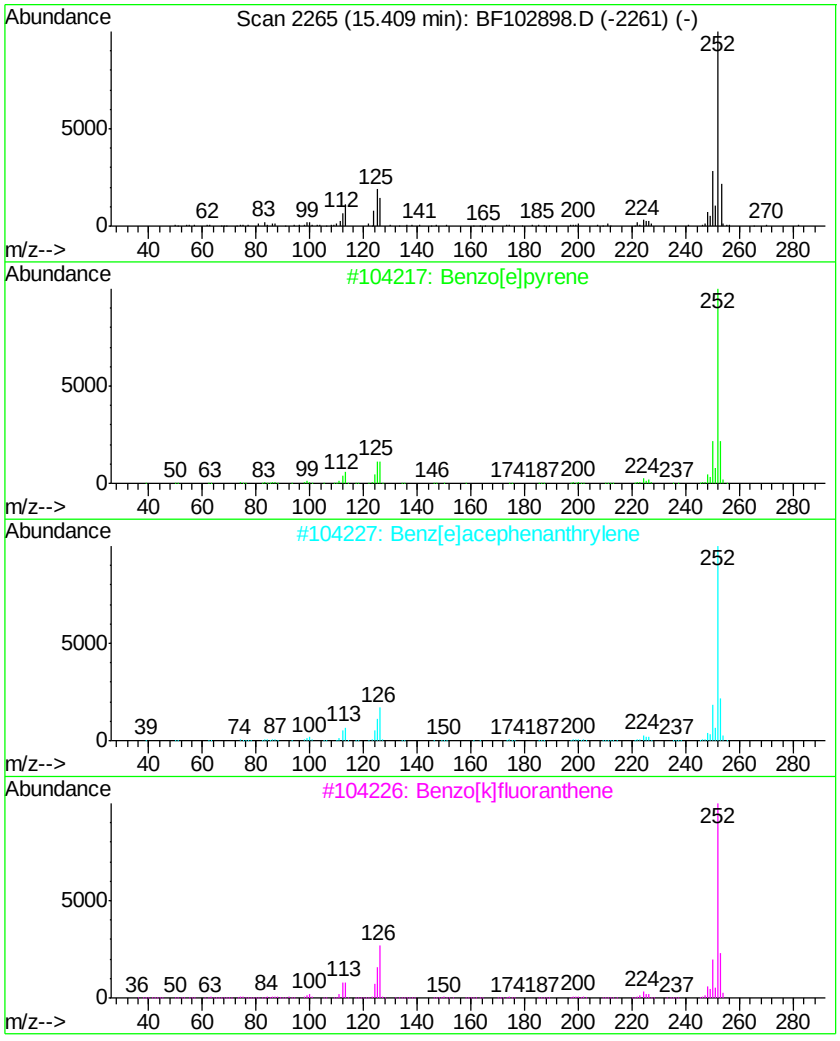
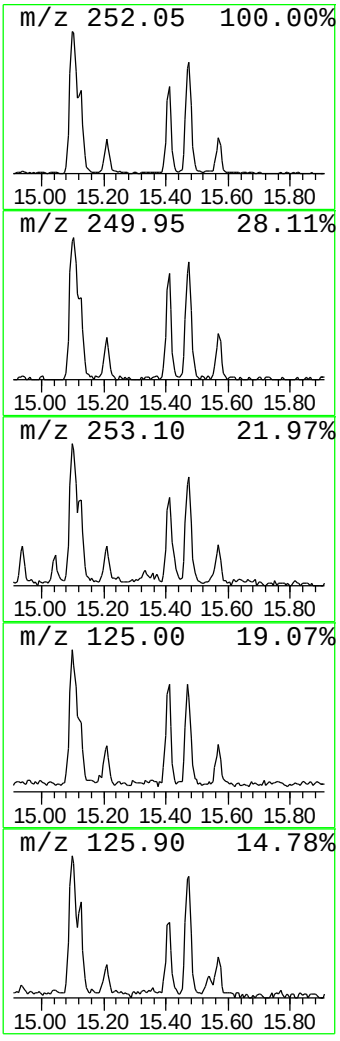
Peak Number 10 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.41	3.47 ng	180461	Perylene-d12	15.54

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





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020918\
Data File : BF102898.D
Acq On : 9 Feb 2018 19:32
Operator : SJ/JU
Sample : J1512-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-2334

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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
Butane, 2-methoxy...	2.17	11.1	ng	621852	1	6.89	1119120	20.0
2-Pentanone, 4-hy...	5.12	2.6	ng	147599	1	6.89	1119120	20.0
unknown6.66	6.66	71.8	ng	4018760	1	6.89	1119120	20.0
Hexadecane	9.85	2.5	ng	162260	3	9.92	1321100	20.0
Dodecane, 2-methy...	10.82	3.5	ng	196846	4	11.41	1113760	20.0
1-Heneicosanol	13.88	5.6	ng	388012	5	14.05	1374820	20.0
Octadecane	14.51	2.9	ng	198065	5	14.05	1374820	20.0
Benzo[e]pyrene	15.41	3.5	ng	180461	6	15.54	1040730	20.0