LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112901.D
Acq On : 7 Mar 2019 00:43
Operator : JU/SJ
Sample : K1705-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-028-SW005-022719

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-BF022719.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	5.345	549	554	557	rBV	4274001	4079596	95.20%	8.311%
2	6.369	723	728	731	rBV	4092605	4203219	98.09%	8.562%
3	6.504	746	751	754	rBV	4246430	4285226	100.00%	8.730%
4	6.734	786	790	793	rBV	1512562	1340690	31.29%	2.731%
5	6.887	812	816	820	rBV	3645032	3314324	77.34%	6.752%
6	7.287	880	884	897	rBV	2657221	2732939	63.78%	5.567%
7	8.010	1003	1007	1014	rBV	1600785	1543830	36.03%	3.145%
8	9.086	1186	1190	1200	rBV	4144398	3827346	89.31%	7.797%
9	9.480	1253	1257	1264	rVB	232754	221056	5.16%	0.450%
10	9.763	1301	1305	1314	rBV	1527809	1557542	36.35%	3.173%
11	10.545	1433	1438	1453	rBV	2346236	2470430	57.65%	5.033%
12	11.233	1552	1555	1558	rBV	1384109	1402030	32.72%	2.856%
13	11.774	1643	1647	1650	rBV2	465278	460901	10.76%	0.939%
14	11.804	1650	1652	1657	rVB	85007	90301	2.11%	0.184%
15	12.051	1692	1694	1701	rVB	43527	44367	1.04%	0.090%
16	12.439	1757	1760	1764	rBV	409524	380655	8.88%	0.775%
17	12.557	1777	1780	1788	rBV3	129873	188069	4.39%	0.383%
18	12.669	1793	1799	1804	rBV	326318	368609	8.60%	0.751%
19	12.816	1820	1824	1831	rVB	3515893	3168840	73.95%	6.455%
20	12.998	1852	1855	1858	rVB	50928	54337	1.27%	0.111%
21	13.063	1858	1866	1869	rBV2	59439	80716	1.88%	0.164%
22	13.098	1869	1872	1875	rBV	44594	46636	1.09%	0.095%
23	13.292	1902	1905	1912	rVB2	56393	83157	1.94%	0.169%
24	13.404	1921	1924	1929	rVB3	40612	45500	1.06%	0.093%
25	13.492	1934	1939	1946	rBV	4202290	4154092	96.94%	8.462%
26	13.610	1955	1959	1962	rBV2	46897	62805	1.47%	0.128%
27	13.727	1973	1979	1986	rBV2	309703	438022	10.22%	0.892%
28	13.863	1996	2002	2004	rBV	1922752	2123059	49.54%	4.325%
29	13.886	2004	2006	2013	rVB	259264	241725	5.64%	0.492%
30	14.045	2029	2033	2036	rBV2	166831	168885	3.94%	0.344%
31	14.280	2071	2073	2077	rVB3	52875	51262	1.20%	0.104%
32	14.345	2081	2084	2091	rBV	267009	346699	8.09%	0.706%
33	14.639	2131	2134	2139	rVB	318250	327006	7.63%	0.666%
34	14.774	2154	2157	2161	rBV2	65297	64734	1.51%	0.132%

LSC Area Percent Report

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Sample : K1705-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-028-SW005-022719

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-BF022719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.863	2169	2172	2175	rBV	240973	336705	7.86%	0.686%
36	14.957	2184	2188	2192	rBV2	399350	466329	10.88%	0.950%
37	15.145	2216	2220	2226	rBV	136503	180317	4.21%	0.367%
38	15.204	2226	2230	2235	rVV	177580	277787	6.48%	0.566%
39	15.262	2235	2240	2245	rVV	1401421	1775054	41.42%	3.616%
40	15.310	2245	2248	2254	rVB	335838	423584	9.88%	0.863%
41	15.715	2312	2317	2323	rBV	317278	464995	10.85%	0.947%
42	16.098	2377	2382	2391	rBV2	379514	803474	18.75%	1.637%
43	16.186	2393	2397	2408	rVB2	139205	267863	6.25%	0.546%
44	16.445	2437	2441	2450	rBV5	65593	124116	2.90%	0.253%

Sum of corrected areas: 49088829

LSC Report - Integrated Chromatogram

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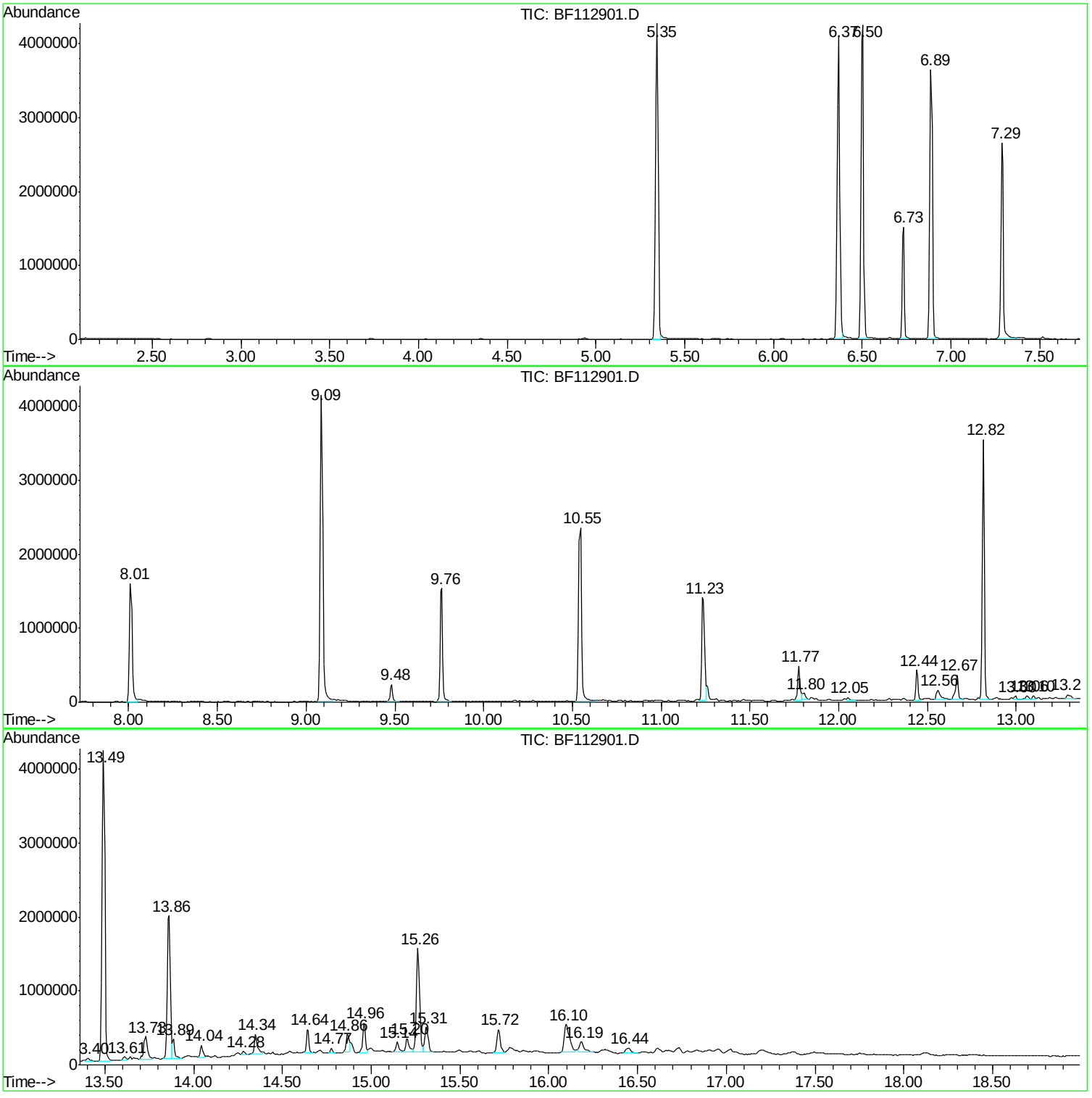
Data File : BF112901.D
Acq On : 7 Mar 2019 00:43
Operator : JU/SJ
Sample : K1705-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EXT-028-SW005-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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\BF030619\
Data File : BF112901.D
Acq On : 7 Mar 2019 00:43
Operator : JU/SJ
Sample : K1705-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-028-SW005-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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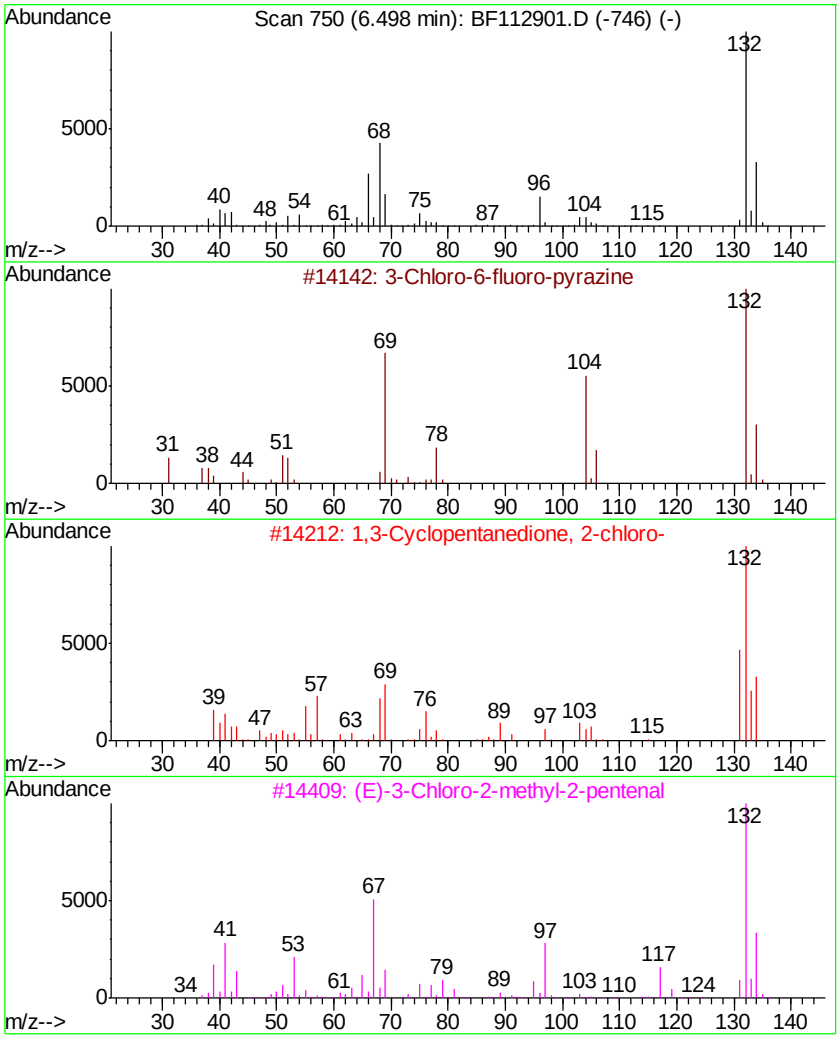
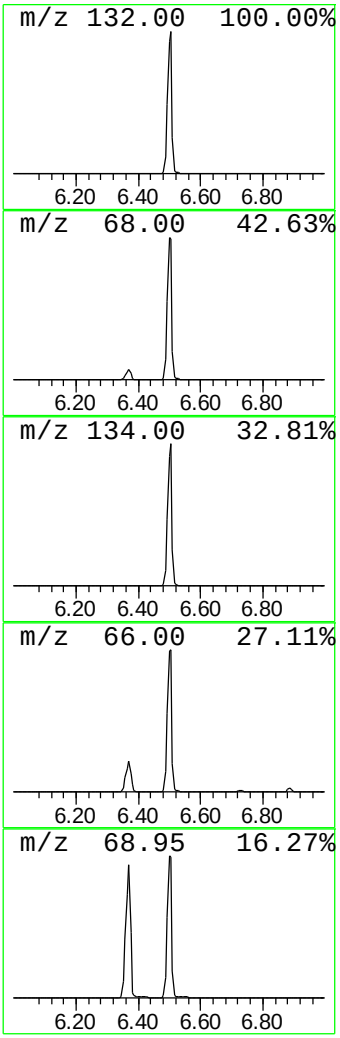
Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	63.93 ng	4285230	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	27
2	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Instrument : BNA_F
ClientSampleId : EXT-028-SW005-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
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TIC Library : C:\DATABASE\NIST11.L
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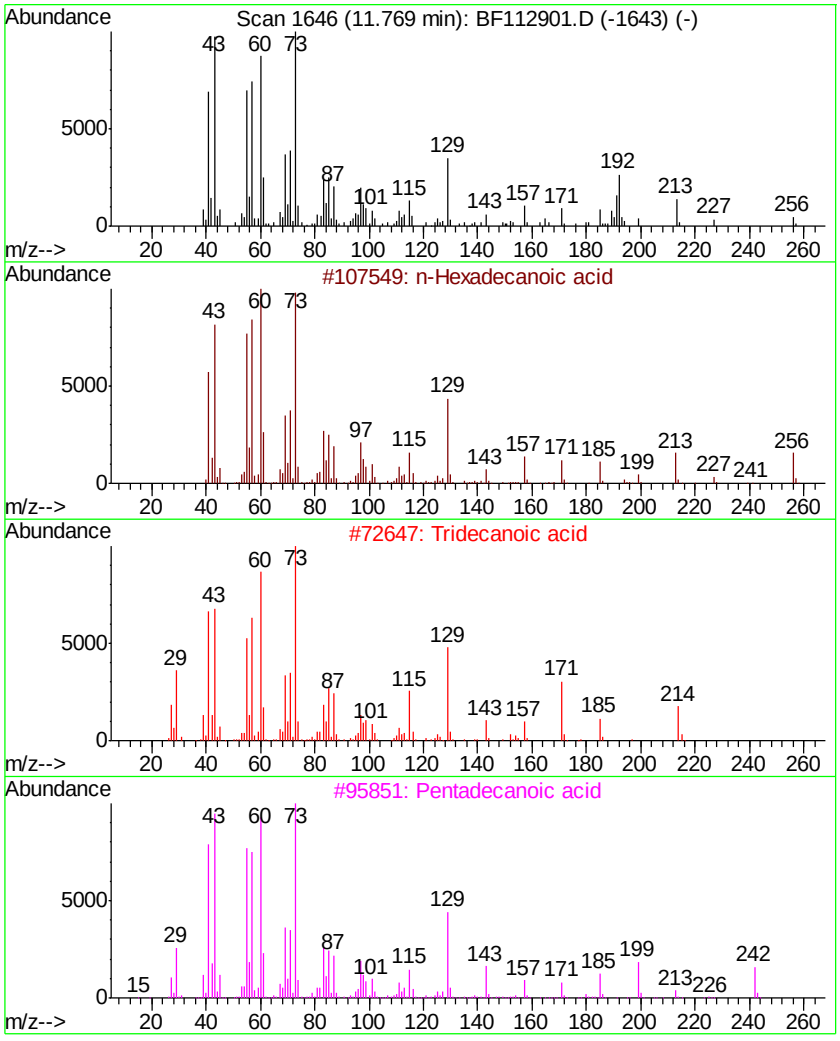
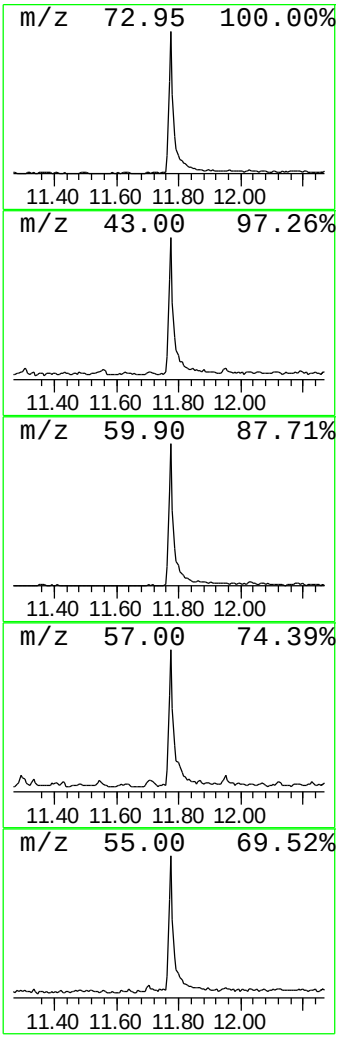
Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	6.57 ng	460901	Phenanthrene-d10	11.23

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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
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Acq On : 7 Mar 2019 00:43
Operator : JU/SJ
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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-028-SW005-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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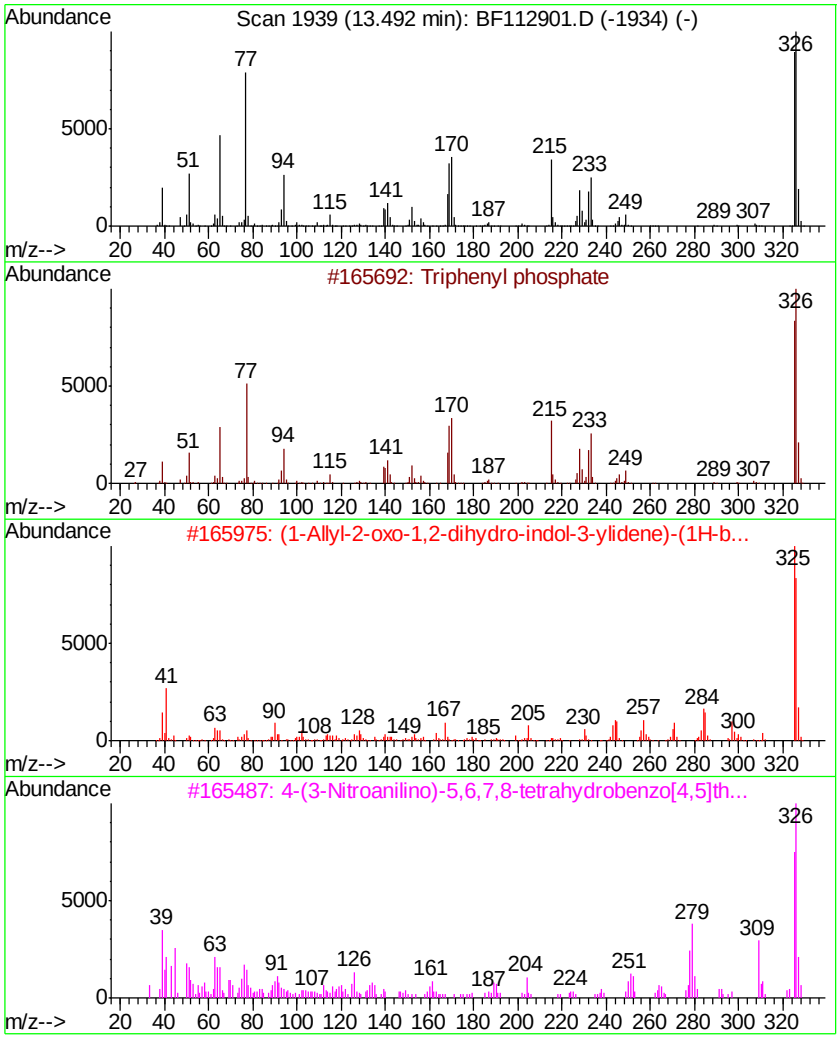
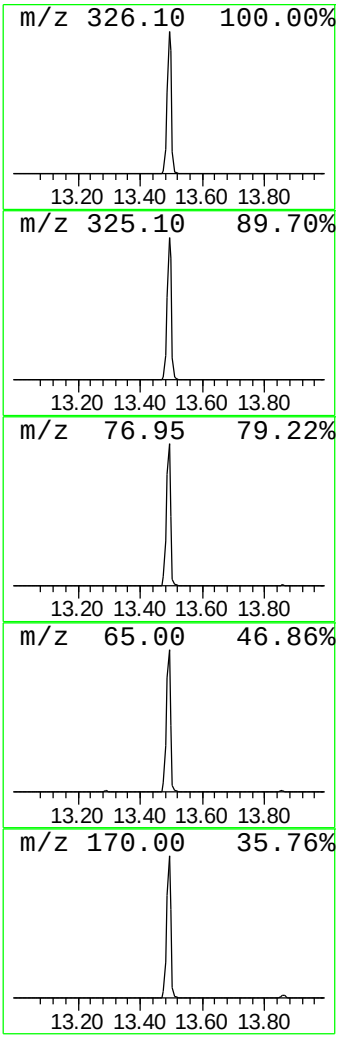
Peak Number 4 Triphenyl phosphate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	39.13 ng	4154090	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenyl phosphate	326	C18H15O4P	000115-86-6	99
2	(1-Allyl-2-oxo-1,2-dihydro-indol...	326	C20H14N4O	1000296-28-1	22
3	4-(3-Nitroanilino)-5,6,7,8-tetra...	326	C16H14N4O2S	313952-58-8	12
4	Coumarin, 3-benzoyl-4-phenyl-	326	C22H14O3	019725-29-2	12
5	(5-Oxo-1-phenyl-4-thiophen-2-ylm...	326	C17H14N2O3S	1000302-22-9	10





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Misc :
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Instrument : BNA_F
ClientSampleId : EXT-028-SW005-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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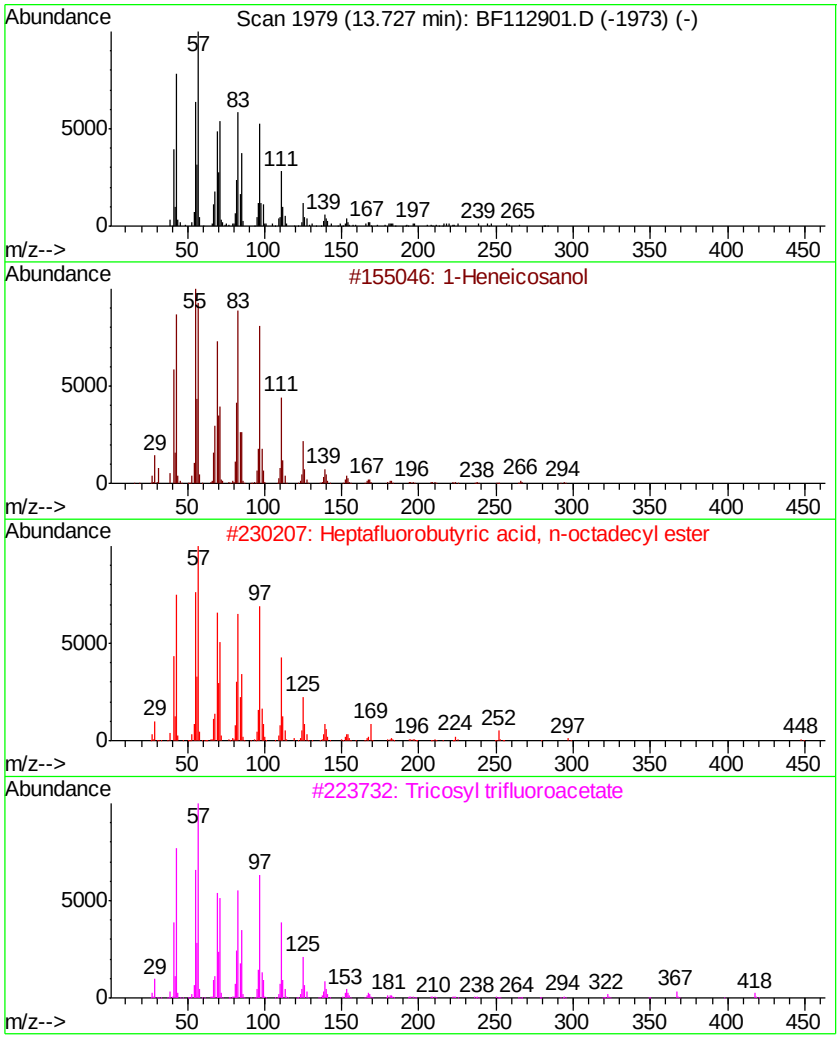
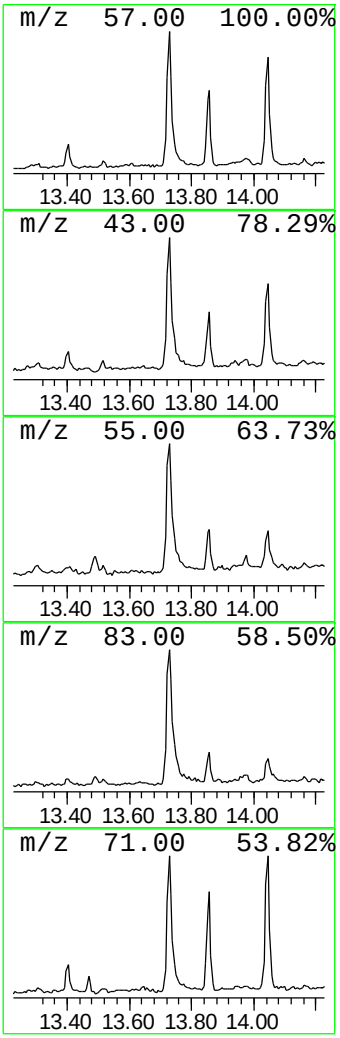
Peak Number 5 1-Heneicosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	4.13 ng	438022	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
3	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91





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Operator : JU/SJ
Sample : K1705-04
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Instrument : BNA_F
ClientSampleId : EXT-028-SW005-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
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TIC Library : C:\DATABASE\NIST11.L
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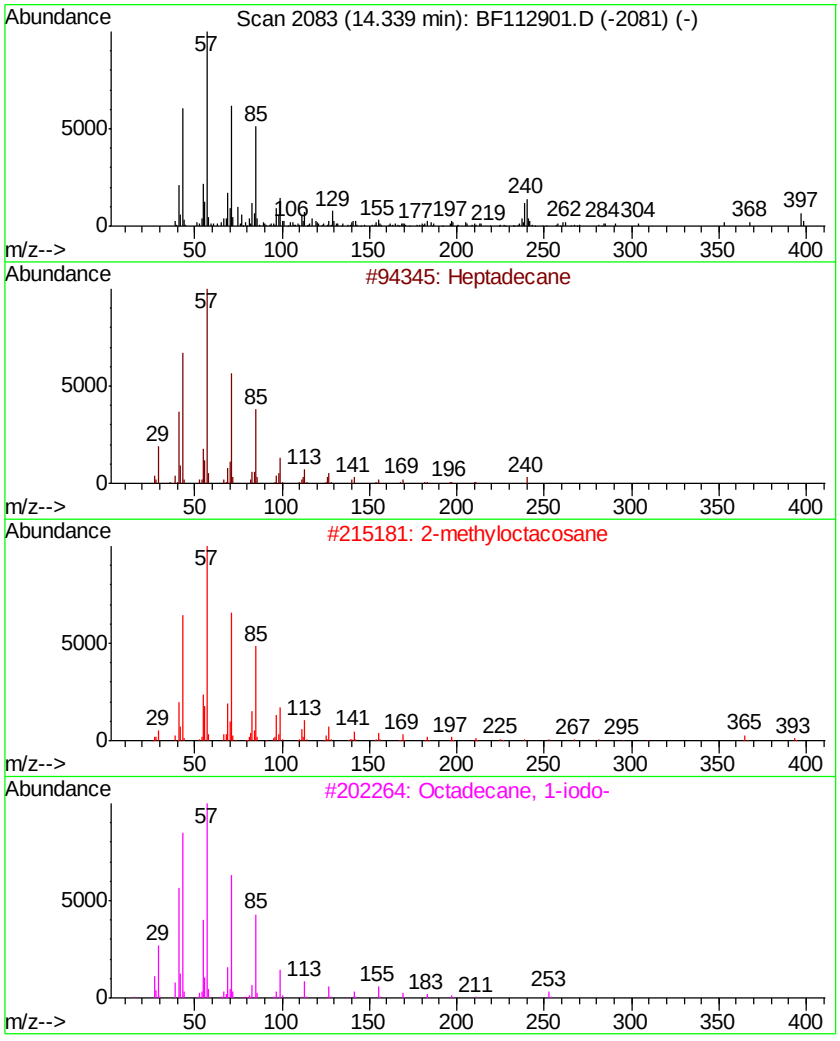
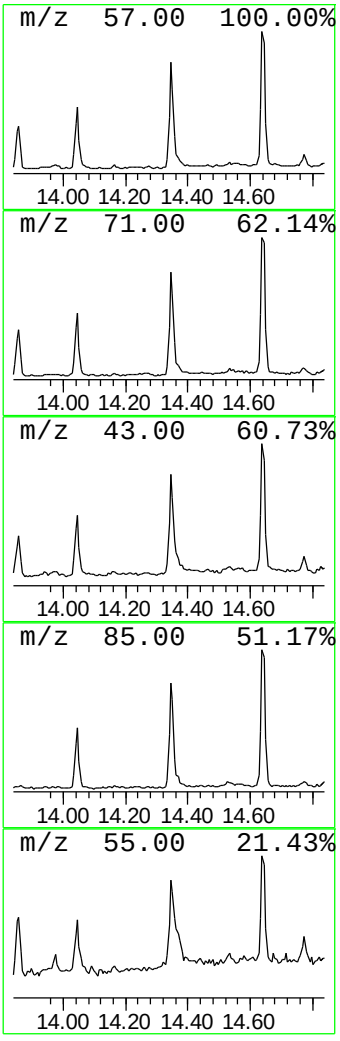
Peak Number 6 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	3.27 ng	346699	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	93
2	2-methyloctacosane	408	C29H60	1000376-72-8	83
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	74
4	Tetracosane	338	C24H50	000646-31-1	74
5	Octadecane	254	C18H38	000593-45-3	74





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Sample : K1705-04
Misc :
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Instrument : BNA_F
ClientSampleId : EXT-028-SW005-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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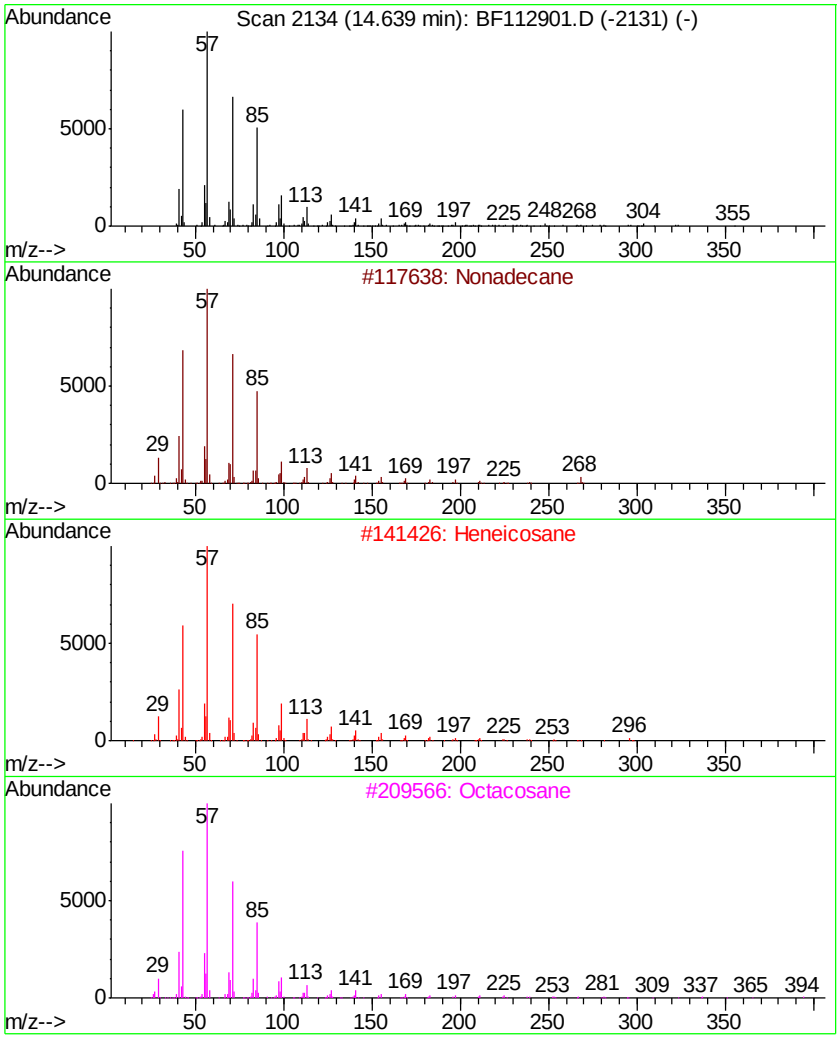
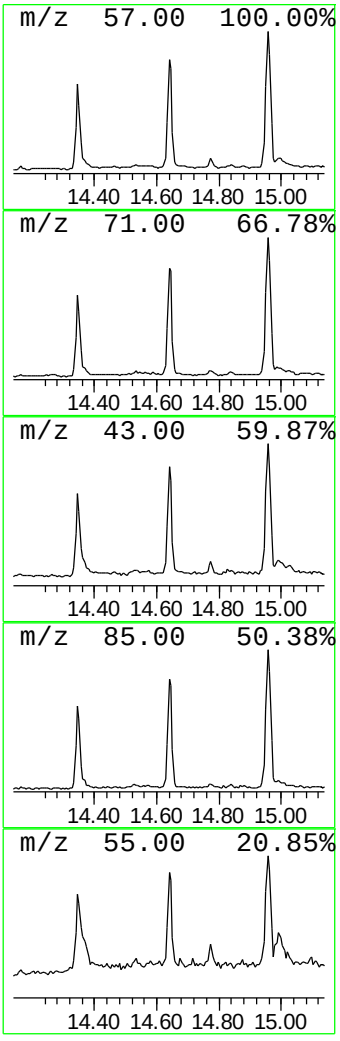
Peak Number 7 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	3.68 ng	327006	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Hexadecane	226	C16H34	000544-76-3	87
5	Octadecane	254	C18H38	000593-45-3	87





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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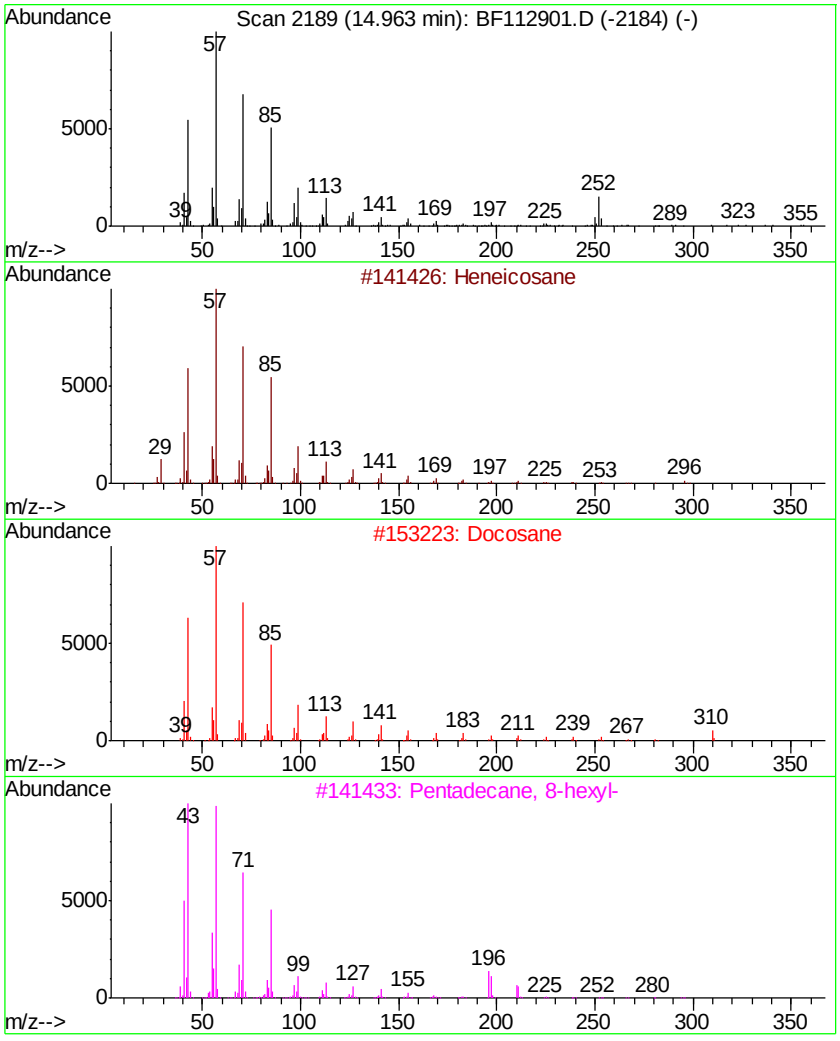
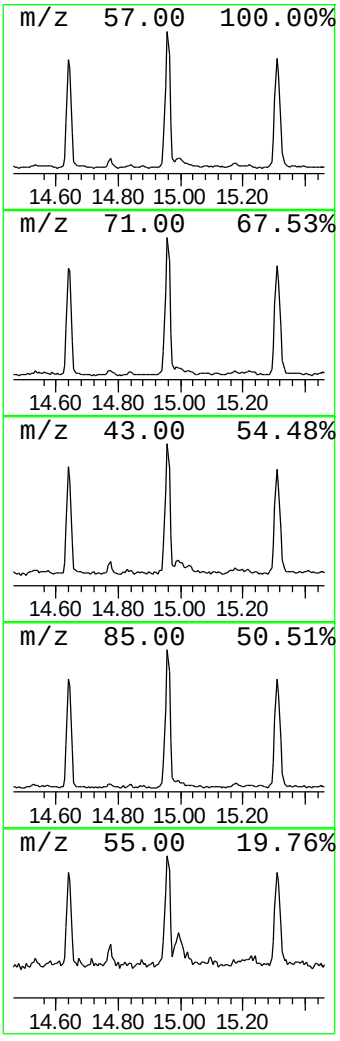
Peak Number 8 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	5.25 ng	466329	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Docosane	310	C22H46	000629-97-0	91
3	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	89
5	Tridecane, 6-propyl-	226	C16H34	055045-10-8	87





Library Search Compound Report

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Data File : BF112901.D
Acq On : 7 Mar 2019 00:43
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Sample : K1705-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-028-SW005-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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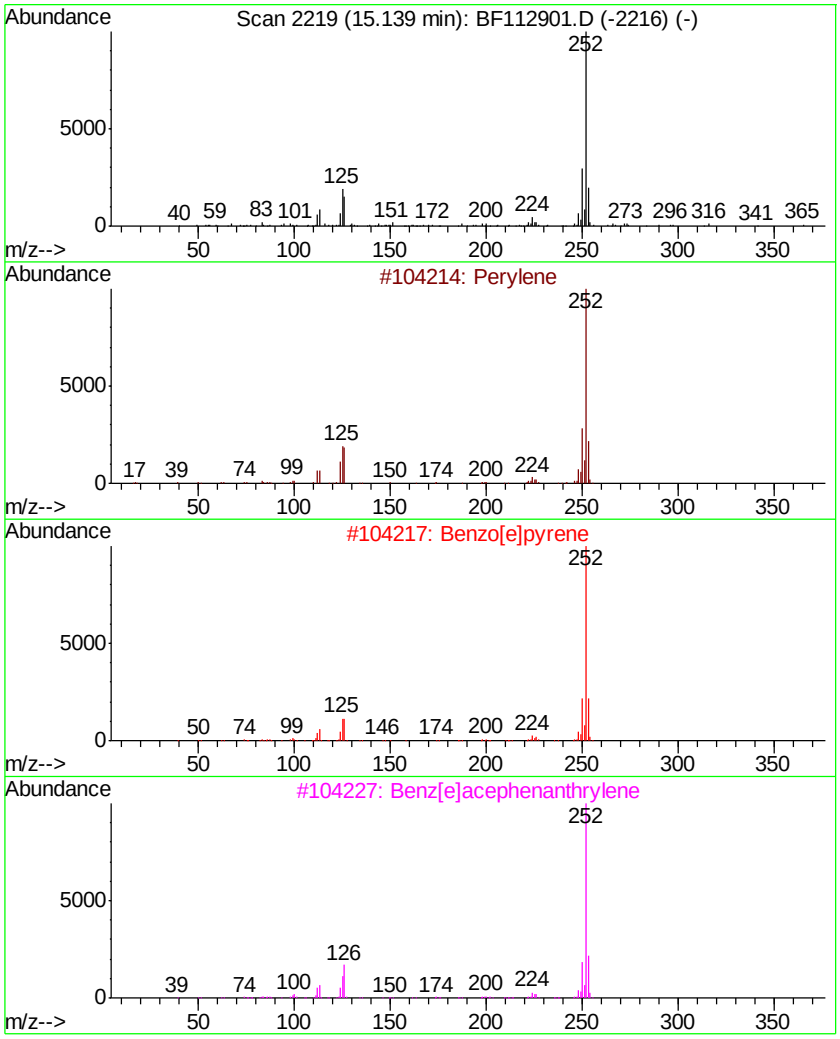
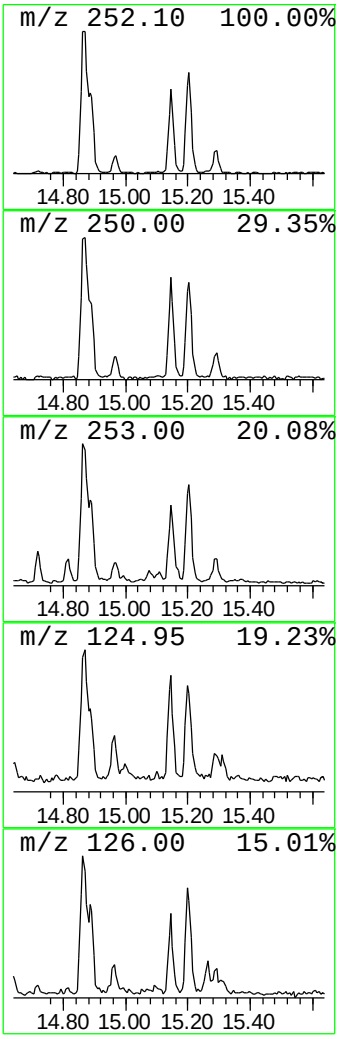
Peak Number 9 Perylene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.14	2.03 ng	180317	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	99
2	Benzo[e]pyrene	252	C20H12	000192-97-2	98
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	98
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	96
5	Benzo[a]pyrene	252	C20H12	000050-32-8	93





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Sample : K1705-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-028-SW005-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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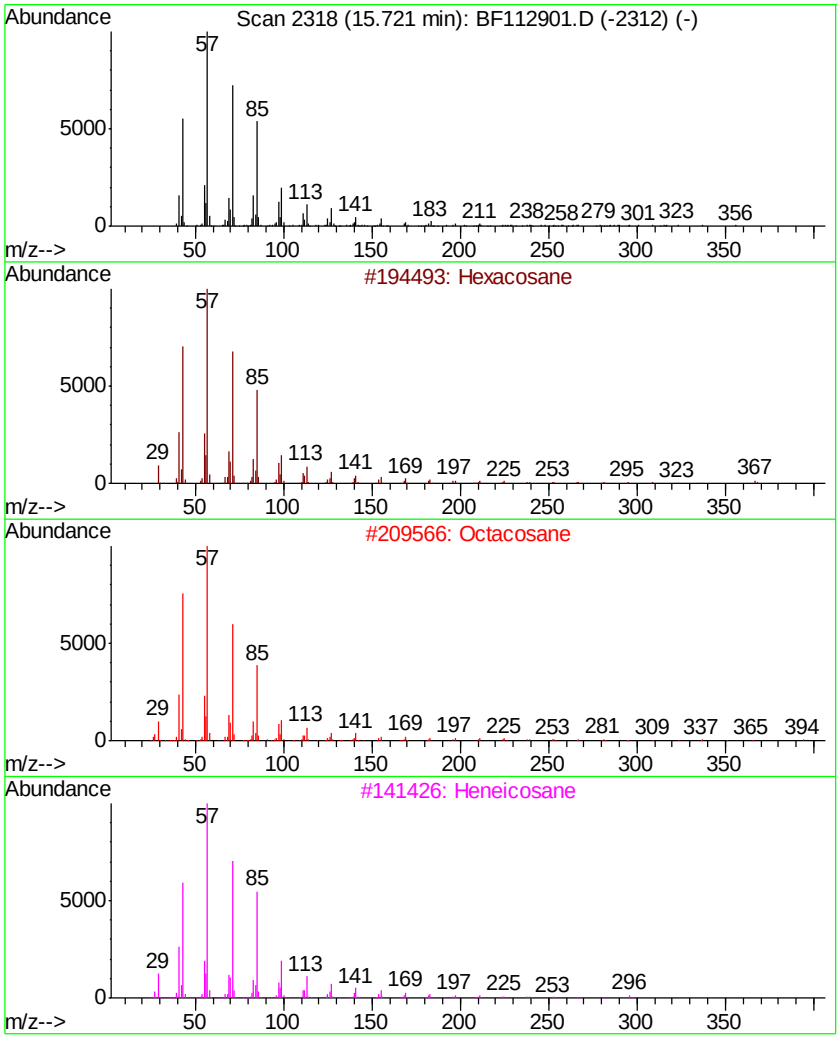
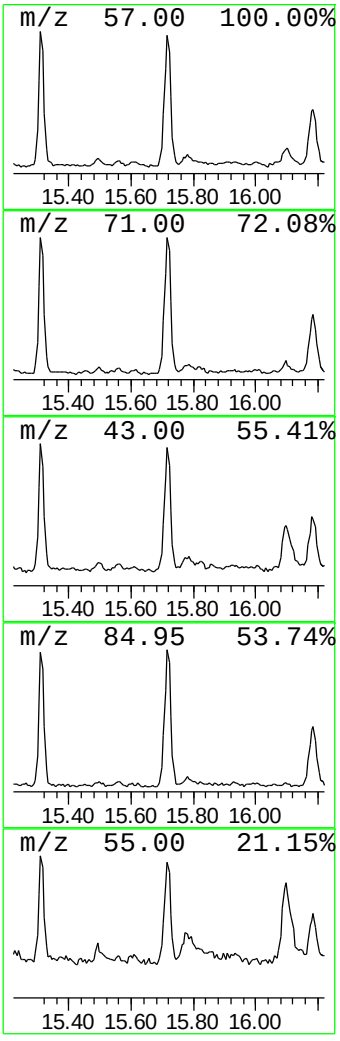
Peak Number 10 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	5.24 ng	464995	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112901.D
Acq On : 7 Mar 2019 00:43
Operator : JU/SJ
Sample : K1705-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-028-SW005-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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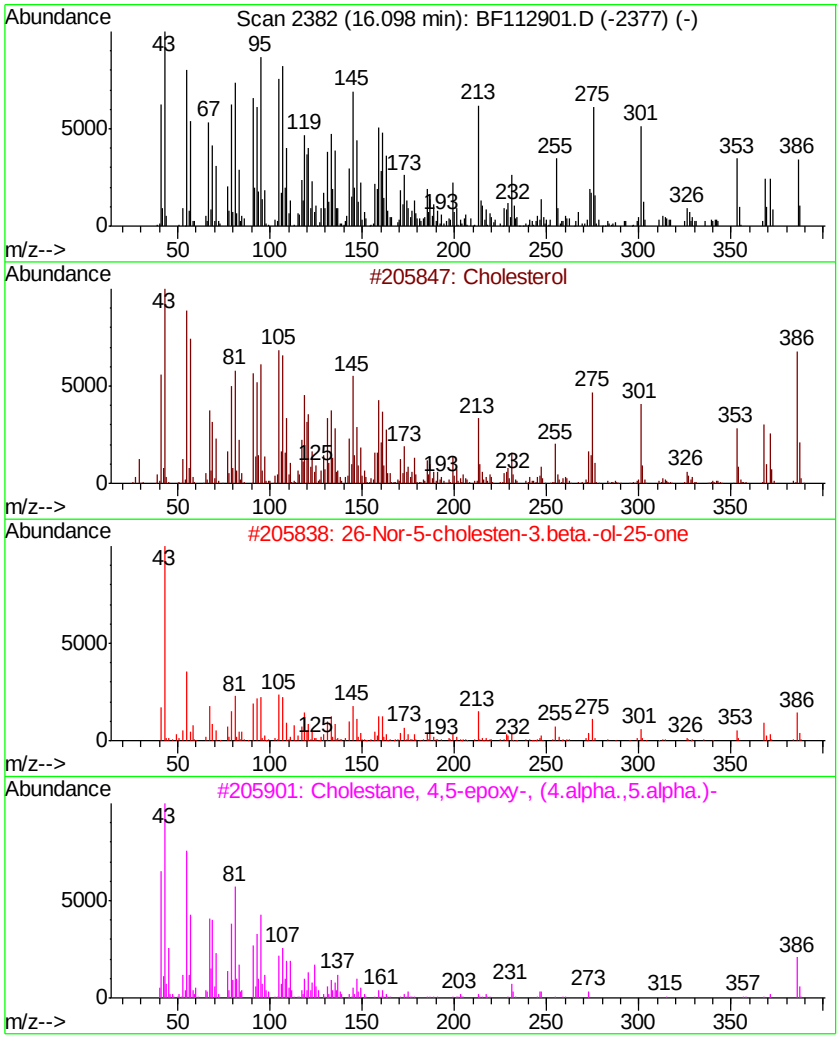
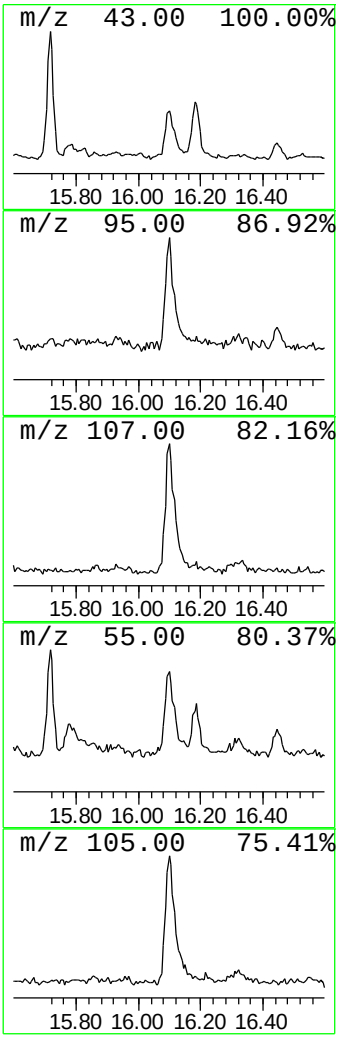
Peak Number 11 Cholesterol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	9.05 ng	803474	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholesterol	386	C27H46O	000057-88-5	99
2	26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	99
3	Cholestane, 4,5-epoxy-, (4.alpha...	386	C27H46O	006079-19-2	50
4	Cholest-5-en-3-ol (3.beta.)-, ac...	428	C29H48O2	000604-35-3	38
5	Cholesta-3,5-diene	368	C27H44	000747-90-0	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030619\
Data File : BF112901.D
Acq On : 7 Mar 2019 00:43
Operator : JU/SJ
Sample : K1705-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EXT-028-SW005-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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	63.9	ng	4285230	1	6.73	1340690	20.0
n-Hexadecanoic acid	11.77	6.6	ng	460901	4	11.23	1402030	20.0
Triphenyl phosphate	13.49	39.1	ng	4154090	5	13.86	2123060	20.0
1-Heneicosanol	13.73	4.1	ng	438022	5	13.86	2123060	20.0
Heptadecane	14.34	3.3	ng	346699	5	13.86	2123060	20.0
Nonadecane	14.64	3.7	ng	327006	6	15.26	1775050	20.0
Heneicosane	14.96	5.3	ng	466329	6	15.26	1775050	20.0
Perylene	15.14	2.0	ng	180317	6	15.26	1775050	20.0
Hexacosane	15.72	5.2	ng	464995	6	15.26	1775050	20.0
Cholesterol	16.10	9.1	ng	803474	6	15.26	1775050	20.0