LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051319\
Data File : BF114240.D
Acq On : 13 May 2019 20:11
Operator : JU/SJ
Sample : K2822-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-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-BF051019.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	5.498	575	580	600	rBV	4362656	4596345	98.40%	9.179%
2	6.510	747	752	755	rBV	4890209	4670936	100.00%	9.328%
3	6.633	769	773	777	rBV	5033124	4610038	98.70%	9.207%
4	6.857	807	811	818	rBV	1588280	1324143	28.35%	2.644%
5	7.010	834	837	841	rBV	3446599	3249220	69.56%	6.489%
6	7.416	902	906	909	rBV	3150470	2863194	61.30%	5.718%
7	8.139	1025	1029	1032	rBV	1729880	1600909	34.27%	3.197%
8	9.210	1207	1211	1221	rBV	4845270	4208272	90.09%	8.404%
9	9.604	1274	1278	1283	rBV	690370	600110	12.85%	1.198%
10	9.892	1323	1327	1335	rVB	2018159	1804561	38.63%	3.604%
11	10.680	1457	1461	1471	rBV	2794273	2866768	61.37%	5.725%
12	10.916	1498	1501	1504	rVB	68600	62870	1.35%	0.126%
13	11.374	1576	1579	1583	rBV	1806602	1760257	37.69%	3.515%
14	11.904	1663	1669	1676	rBV	925030	930500	19.92%	1.858%
15	12.592	1783	1786	1791	rBV	89529	94764	2.03%	0.189%
16	12.686	1799	1802	1808	rBV	204102	222535	4.76%	0.444%
17	12.821	1822	1825	1828	rVB2	59402	55184	1.18%	0.110%
18	12.957	1844	1848	1852	rBV	3488312	3282650	70.28%	6.556%
19	13.163	1880	1883	1886	rBV2	149778	172713	3.70%	0.345%
20	13.762	1971	1985	1986	rBV	1543086	4211624	90.17%	8.411%
21	13.851	1997	2000	2008	rVB	1306880	1538683	32.94%	3.073%
22	14.021	2026	2029	2033	rBV	1435532	1366207	29.25%	2.728%
23	14.180	2054	2056	2059	rVB	121607	90232	1.93%	0.180%
24	14.504	2107	2111	2117	rVB2	688910	876054	18.76%	1.750%
25	14.804	2159	2162	2170	rVB	281627	337089	7.22%	0.673%
26	15.145	2216	2220	2223	rBV	485799	536801	11.49%	1.072%
27	15.521	2279	2284	2292	rBV2	1218074	1626218	34.82%	3.248%
28	15.962	2355	2359	2363	rVB	377837	514281	11.01%	1.027%

Sum of corrected areas: 50073158

LSC Report - Integrated Chromatogram

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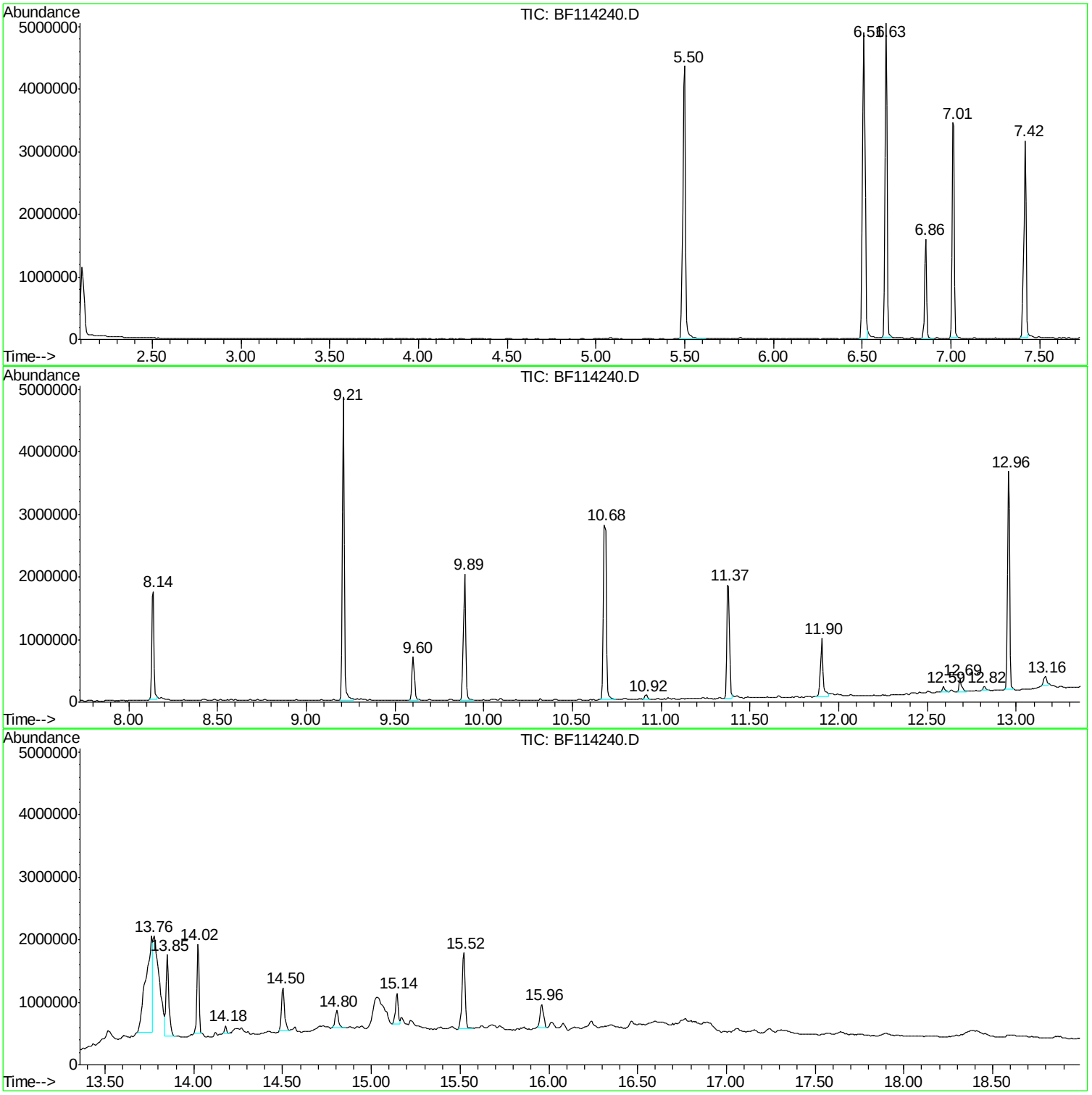
Instrument : BNA_F
ClientSampleId : S-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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

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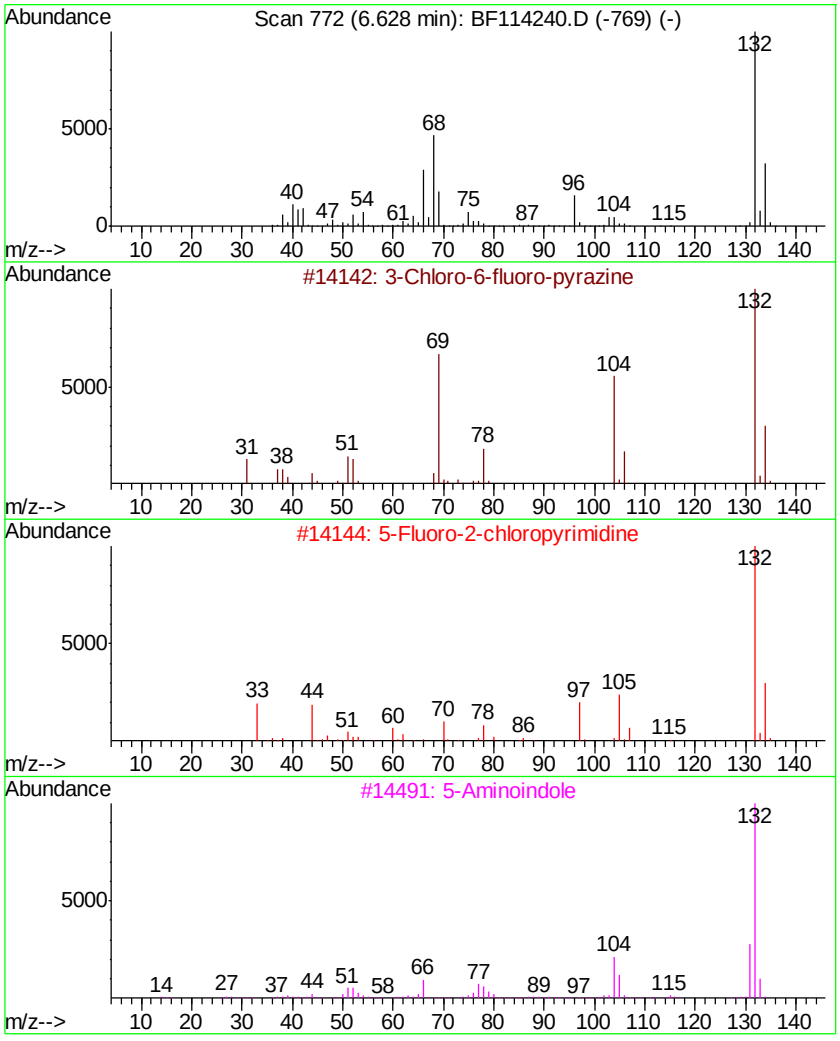
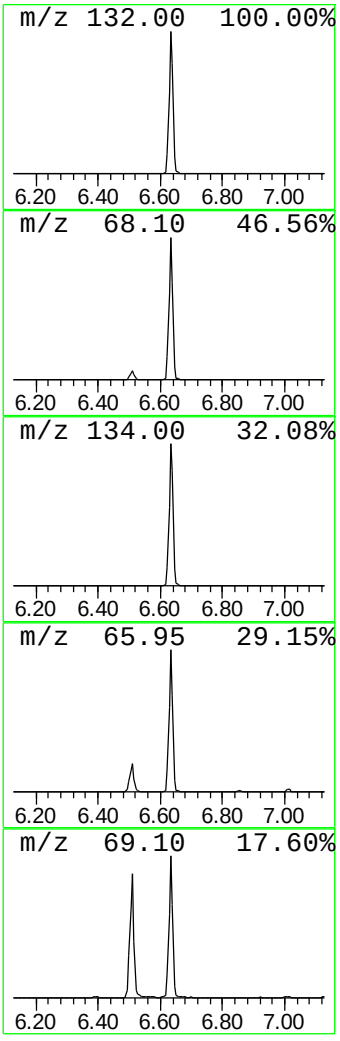
Peak Number 1 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	69.63 ng	4610040	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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Misc :
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Instrument : BNA_F
ClientSampleId : S-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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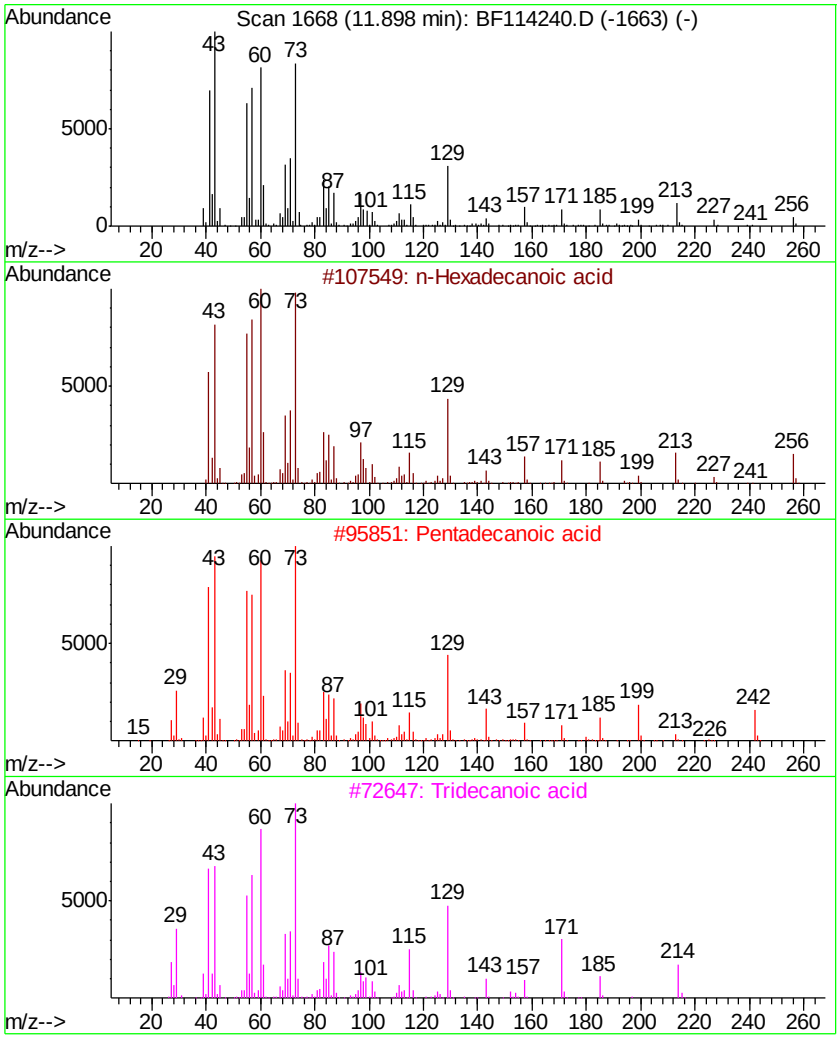
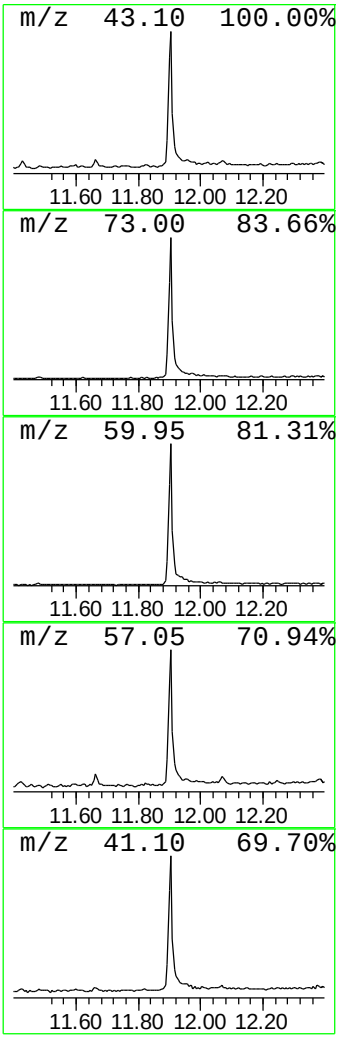
Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	10.57 ng	930500	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	92
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





Library Search Compound Report

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Sample : K2822-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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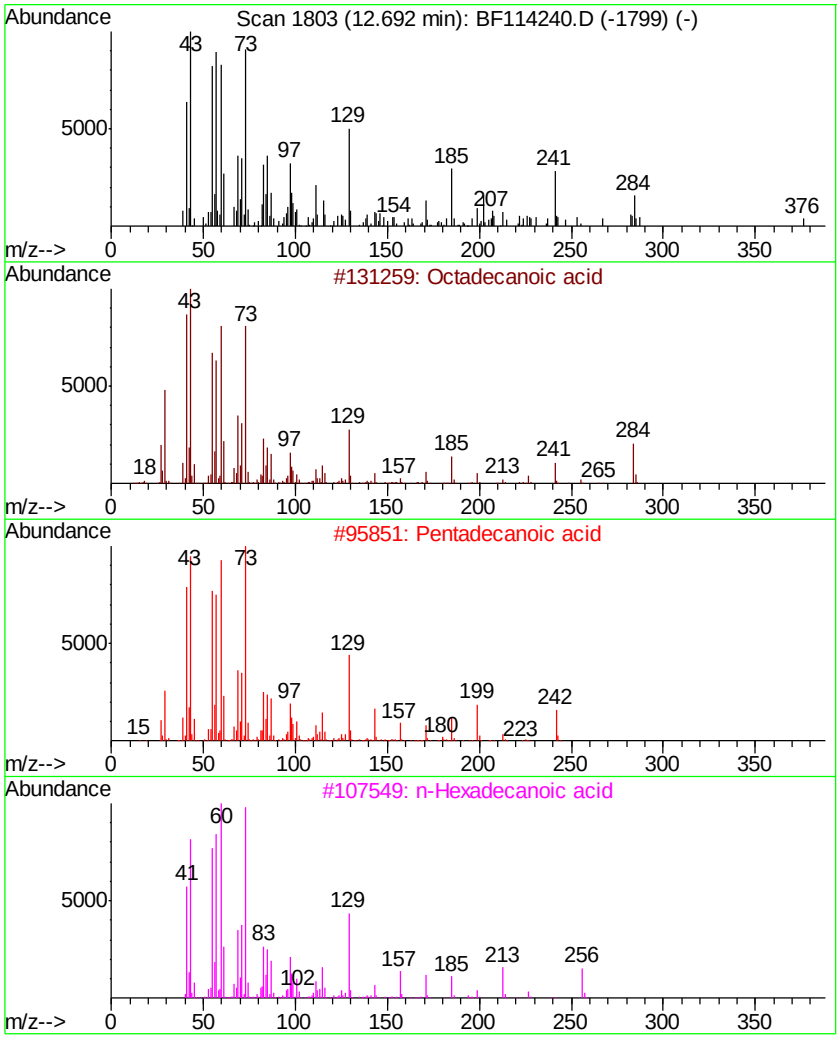
TIC Integration Parameters: LSCINT.P

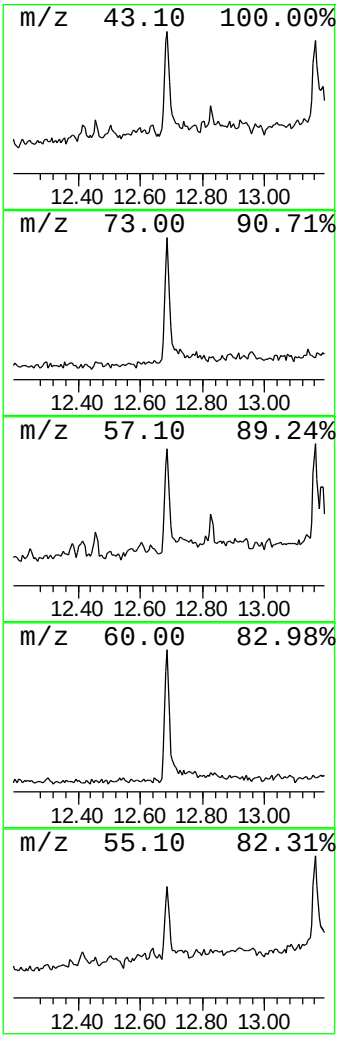
****

Peak Number 4 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.69	2.53 ng	222535	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





Library Search Compound Report

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Sample : K2822-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

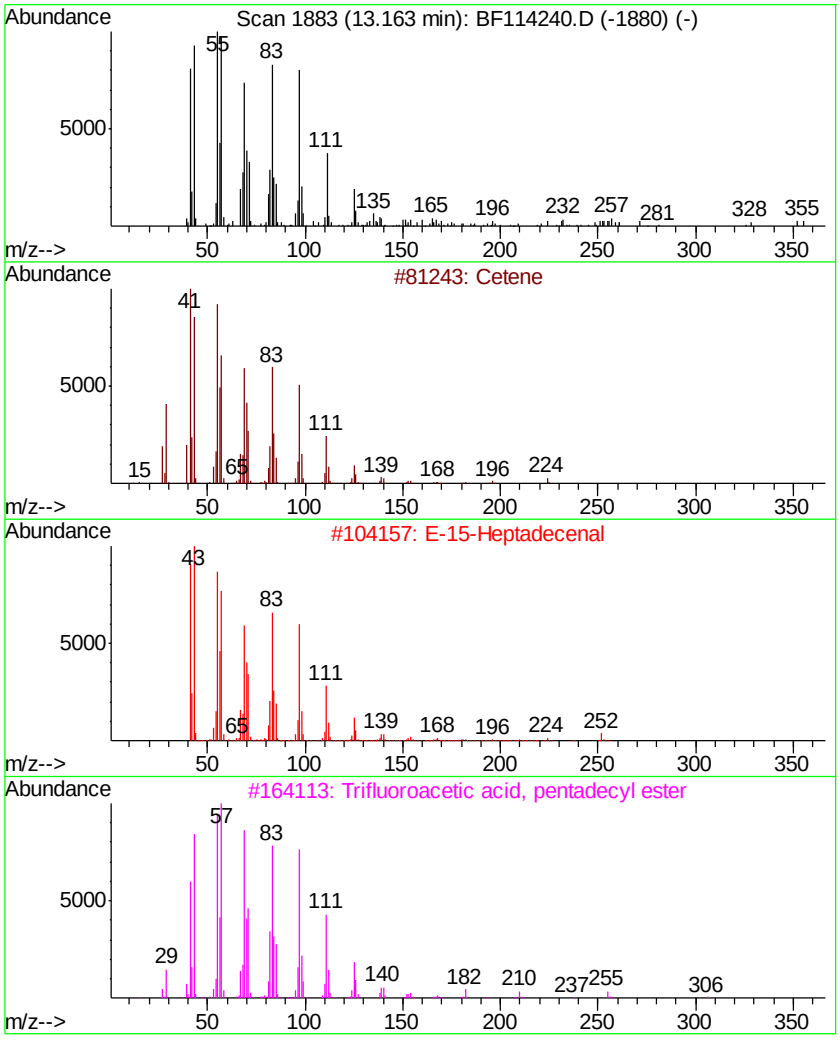
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

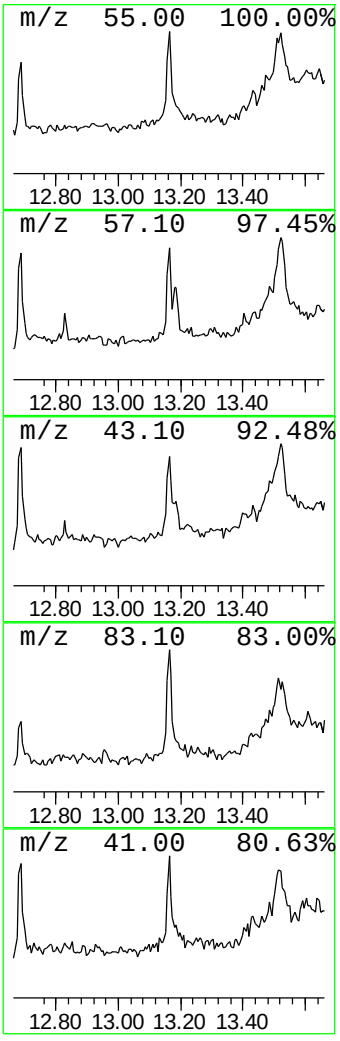
****

Peak Number 5 Cetene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.16	2.53 ng	172713	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cetene	224	C16H32	000629-73-2	96
2	E-15-Heptadecenal	252	C17H32O	1000130-97-9	95
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	91
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	90





Library Search Compound Report

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Sample : K2822-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-3

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

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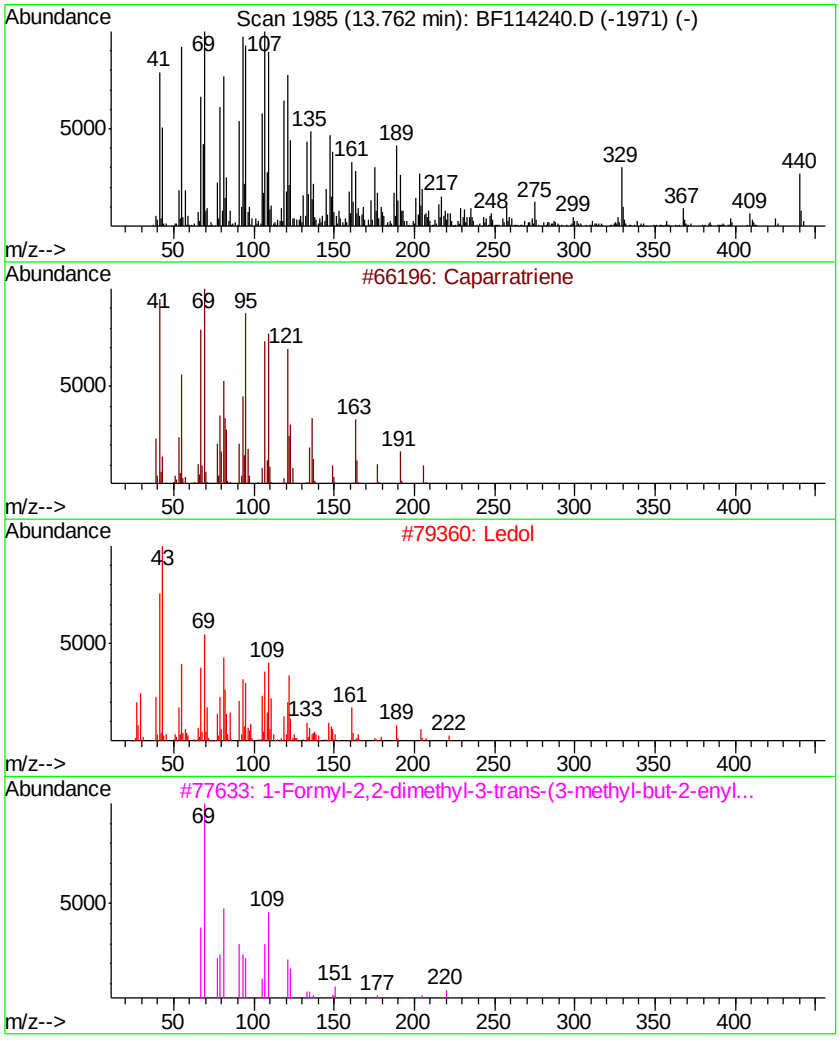
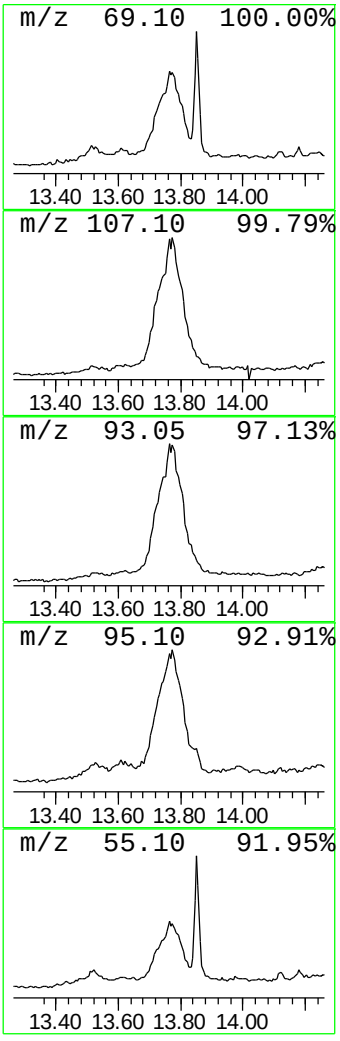
Peak Number 6 Caparratriene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	61.65 ng	4211620	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caparratriene	206	C15H26	1000374-08-7	58
2	Ledol	222	C15H26O	000577-27-5	43
3	1-Formyl-2,2-dimethyl-3-trans-(3...	220	C15H24O	1000144-09-7	43
4	2-Cyclohexene-1-carboxaldehyde, ...	220	C15H24O	056772-07-7	42
5	1,4-Methanoazulene-9-methanol, d...	222	C15H26O	001139-17-9	41





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Misc :
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Instrument : BNA_F
ClientSampleId : S-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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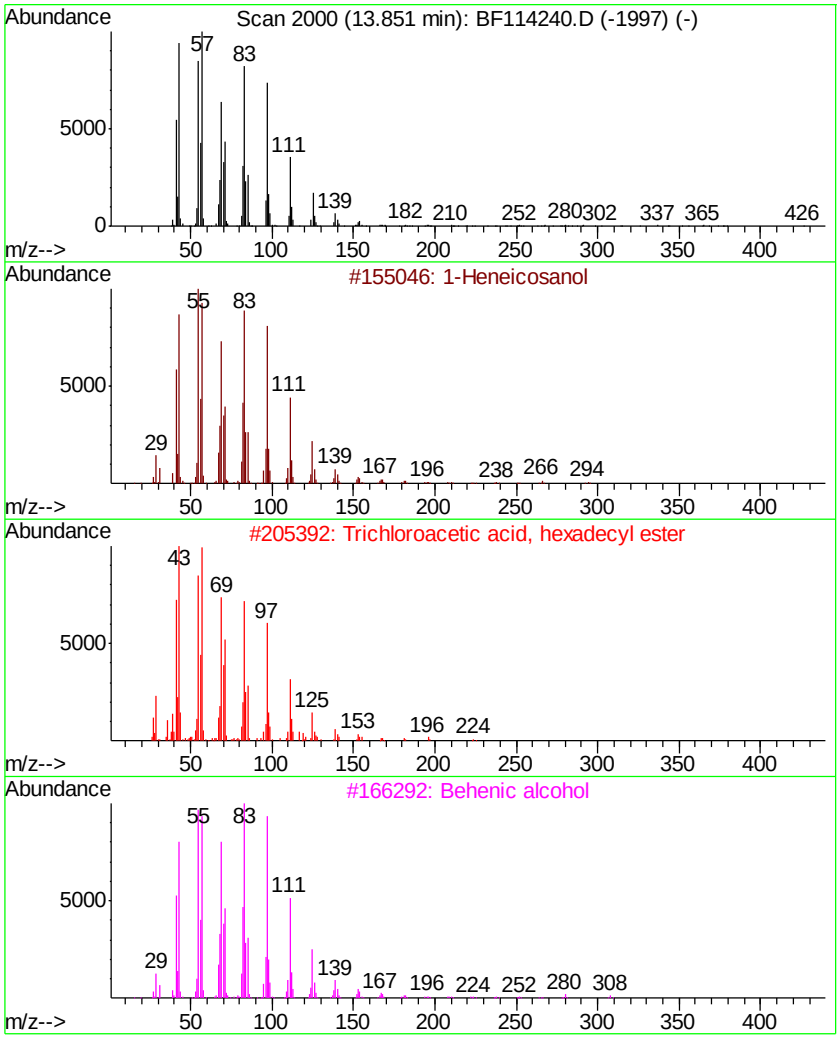
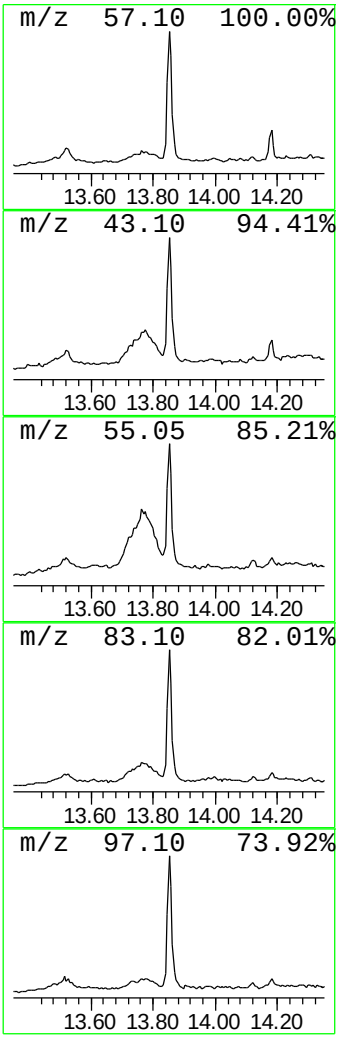
****

Peak Number 7 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	22.52 ng	1538680	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	Cyclotetracosane	336	C24H48	000297-03-0	91
5	1-Nonadecene	266	C19H38	018435-45-5	91





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

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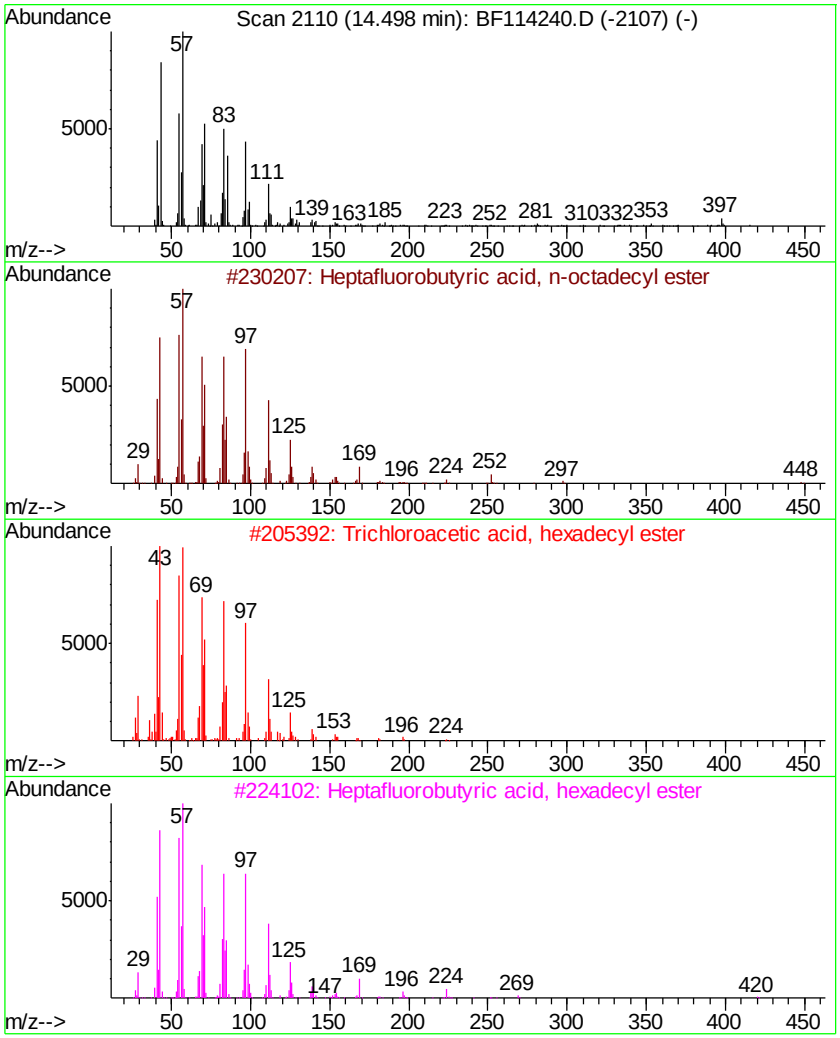
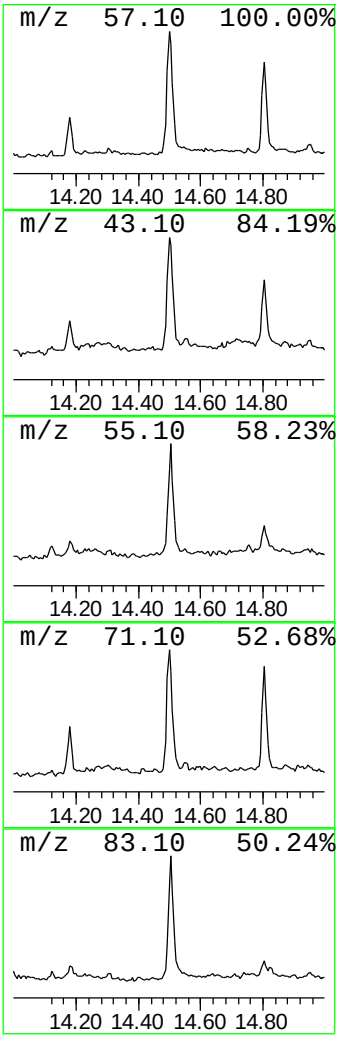
Peak Number 8 Heptafluorobutyric acid, n-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	12.82 ng	876054	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94





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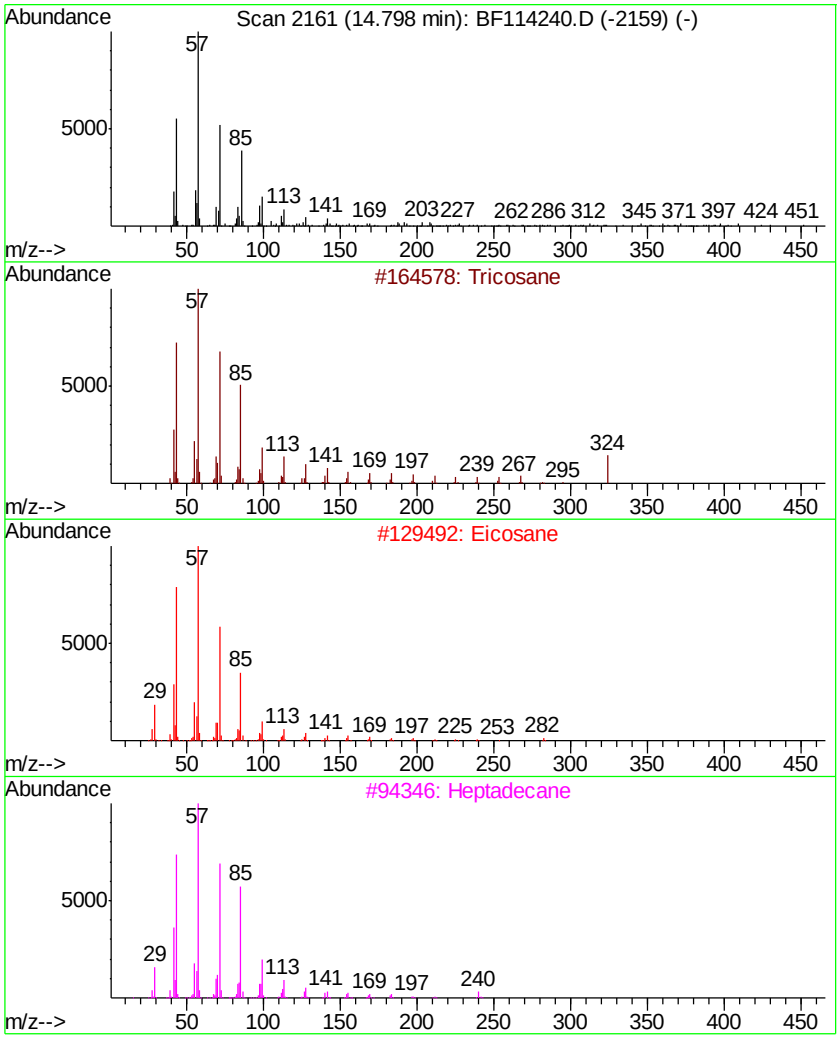
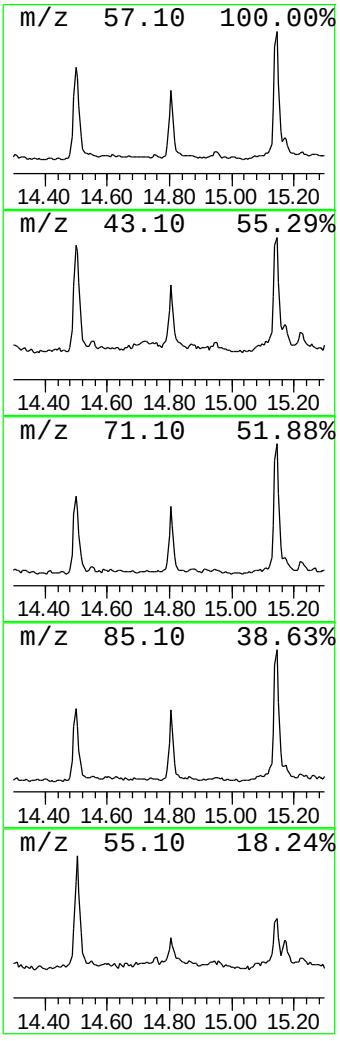
****

Peak Number 9 Tricosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	4.15 ng	337089	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Heptadecane	240	C17H36	000629-78-7	80
4	Hexadecane	226	C16H34	000544-76-3	80
5	Pentacosane	352	C25H52	000629-99-2	72





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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

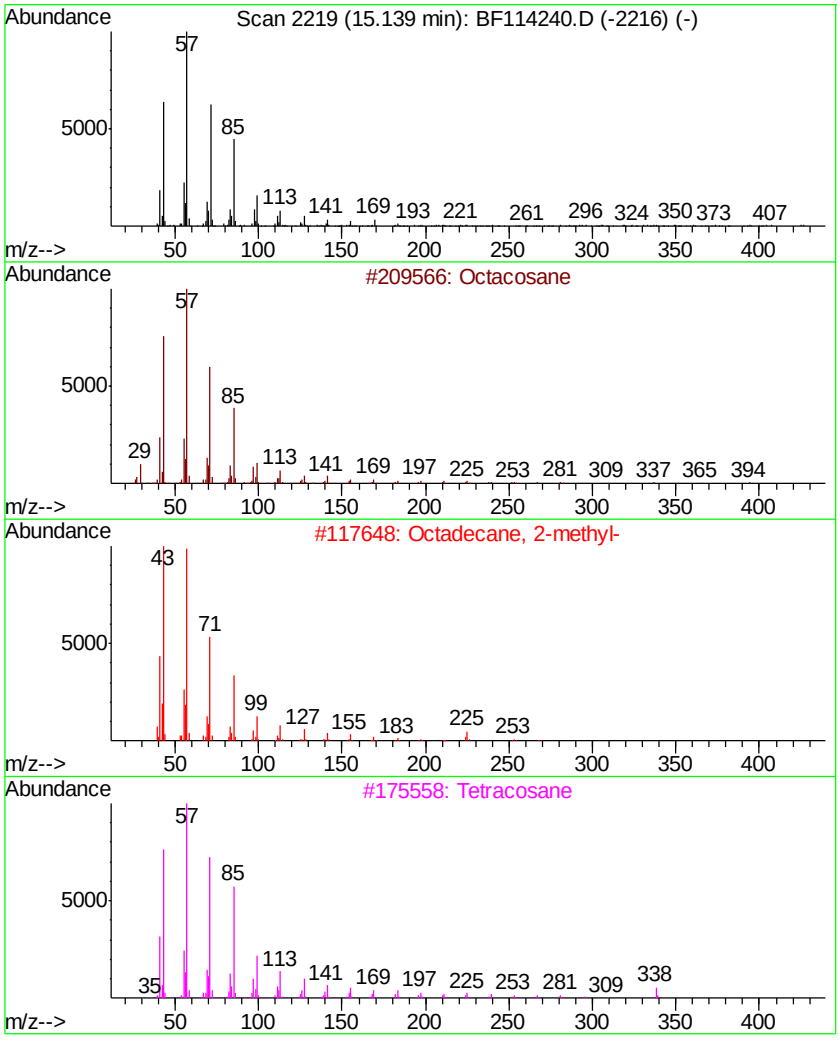
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

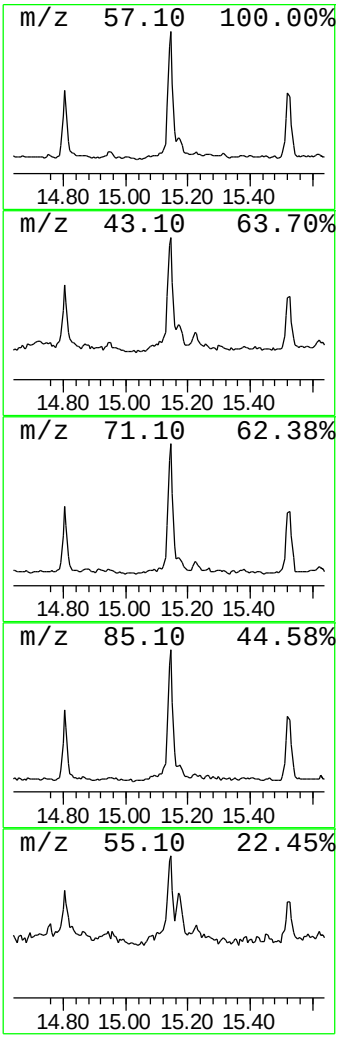
****

Peak Number 10 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.14	6.60 ng	536801	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	99
2	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
3	Tetracosane	338	C24H50	000646-31-1	93
4	Heptacosane	380	C27H56	000593-49-7	90
5	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	87





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Misc :
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Instrument : BNA_F
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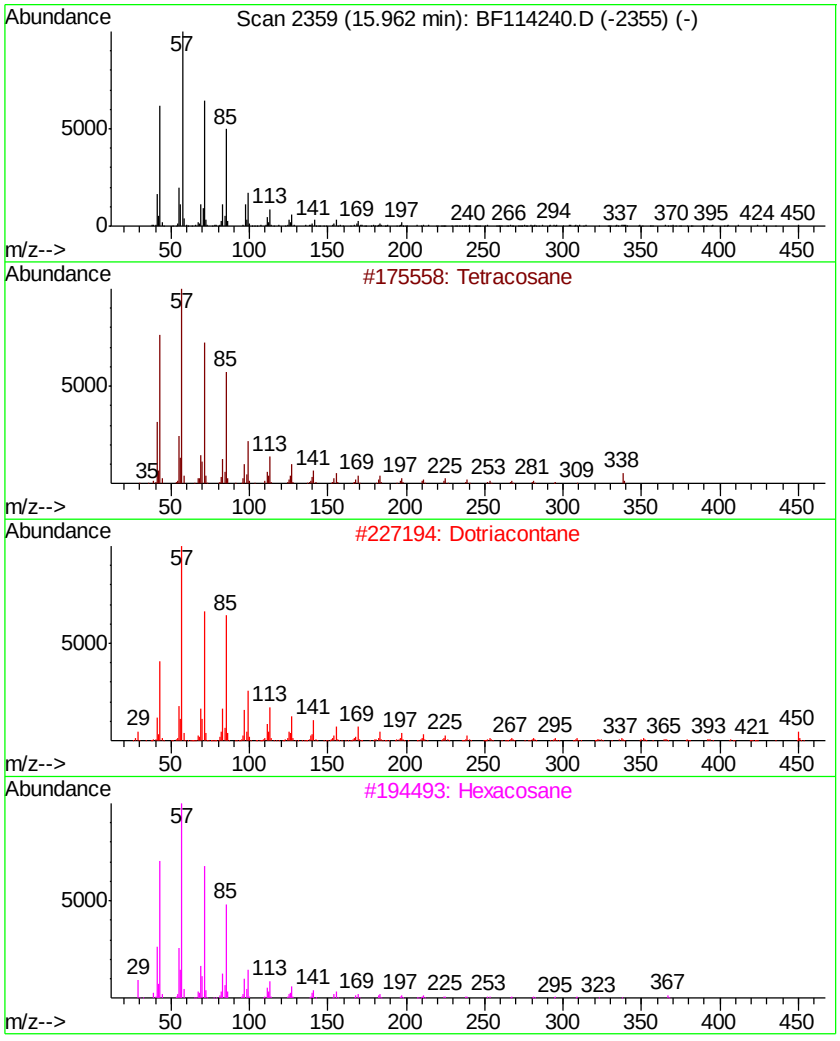
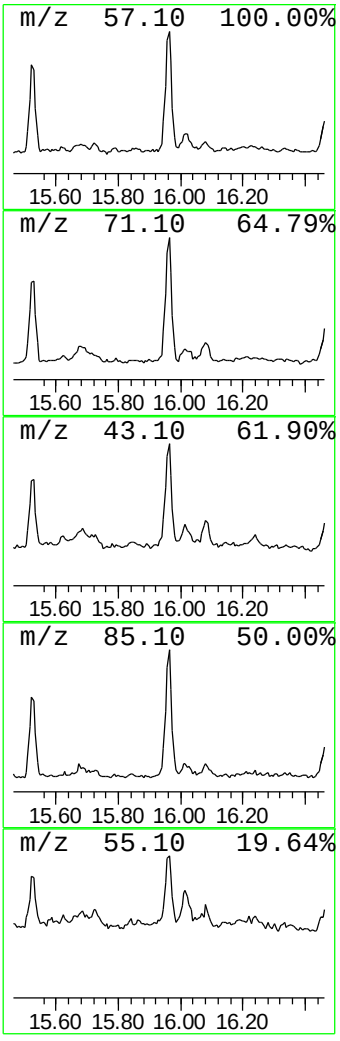
Peak Number 11 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	6.32 ng	514281	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	93
2	Dotriacontane	451	C32H66	000544-85-4	86
3	Hexacosane	366	C26H54	000630-01-3	86
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83
5	Octacosane	394	C28H58	000630-02-4	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051319\
Data File : BF114240.D
Acq On : 13 May 2019 20:11
Operator : JU/SJ
Sample : K2822-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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
unknown6.63	6.63	69.6	ng	4610040	1	6.86	1324140	20.0
n-Hexadecanoic acid	11.90	10.6	ng	930500	4	11.38	1760260	20.0
Octadecanoic acid	12.69	2.5	ng	222535	4	11.38	1760260	20.0
Cetene	13.16	2.5	ng	172713	5	14.02	1366210	20.0
Caparratriene	13.76	61.6	ng	4211620	5	14.02	1366210	20.0
1-Heneicosanol	13.85	22.5	ng	1538680	5	14.02	1366210	20.0
Heptafluorobutyri...	14.50	12.8	ng	876054	5	14.02	1366210	20.0
Tricosane	14.80	4.2	ng	337089	6	15.52	1626220	20.0
Octacosane	15.14	6.6	ng	536801	6	15.52	1626220	20.0
Tetracosane	15.96	6.3	ng	514281	6	15.52	1626220	20.0