LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031319\
Data File : BF113042.D
Acq On : 13 Mar 2019 21:44
Operator : JU/SJ
Sample : K1870-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1

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: BF113041.D

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.334	548	552	570	rBV	1440403	1430150	79.74%	5.483%
2	6.175	690	695	699	rVB	41748	37964	2.12%	0.146%
3	6.363	724	727	742	rBV	1567155	1607275	89.61%	6.162%
4	6.498	746	750	753	rBV	1808949	1598118	89.10%	6.127%
5	6.728	785	789	792	rBV	972466	878132	48.96%	3.366%
6	6.881	811	815	819	rBV	1520755	1208906	67.40%	4.634%
7	7.281	879	883	892	rBV	1045346	958226	53.42%	3.673%
8	7.751	960	963	967	rVB	182253	156915	8.75%	0.602%
9	8.010	1003	1007	1012	rBV	1146188	1127806	62.88%	4.324%
10	8.051	1012	1014	1033	rVB2	29149	85654	4.78%	0.328%
11	9.080	1185	1189	1199	rBV	2073228	1793603	100.00%	6.876%
12	9.422	1241	1247	1249	rBV2	30288	27693	1.54%	0.106%
13	9.475	1252	1256	1262	rVV	159499	139982	7.80%	0.537%
14	9.757	1300	1304	1308	rBV	1624143	1428076	79.62%	5.475%
15	9.963	1336	1339	1343	rBV2	15359	22824	1.27%	0.087%
16	10.275	1386	1392	1394	rBV3	34430	35525	1.98%	0.136%
17	10.539	1433	1437	1448	rBV	1557640	1438076	80.18%	5.513%
18	10.845	1483	1489	1493	rBV8	12726	24664	1.38%	0.095%
19	10.910	1496	1500	1506	rBV7	21800	41846	2.33%	0.160%
20	11.116	1527	1535	1536	rBV6	19840	40444	2.25%	0.155%
21	11.192	1545	1548	1551	rBV4	20728	25900	1.44%	0.099%
22	11.233	1551	1555	1558	rVV	1779282	1598860	89.14%	6.129%
23	11.257	1558	1559	1562	rVV	230502	136508	7.61%	0.523%
24	11.304	1565	1567	1572	rVB	62221	62465	3.48%	0.239%
25	11.698	1630	1634	1637	rBV2	41436	54980	3.07%	0.211%
26	11.733	1637	1640	1643	rVV	50876	53372	2.98%	0.205%
27	11.769	1643	1646	1656	rVV2	449192	518442	28.91%	1.988%
28	11.845	1656	1659	1661	rBV	50154	48331	2.69%	0.185%
29	12.027	1687	1690	1692	rBV	24997	23630	1.32%	0.091%
30	12.051	1692	1694	1698	rVB3	20752	20875	1.16%	0.080%
31	12.280	1730	1733	1735	rBV2	32297	28035	1.56%	0.107%
32	12.363	1744	1747	1754	rVB4	30568	44954	2.51%	0.172%
33	12.439	1756	1760	1764	rBV	419757	385845	21.51%	1.479%
34	12.551	1776	1779	1790	rBV3	137151	201153	11.22%	0.771%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031319\
Data File : BF113042.D
Acq On : 13 Mar 2019 21:44
Operator : JU/SJ
Sample : K1870-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1

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	12.663	1793	1798	1802	rBV	359446	384331	21.43%	1.473%
36	12.739	1808	1811	1816	rVB	98347	94866	5.29%	0.364%
37	12.810	1819	1823	1829	rVB	1902225	1719398	95.86%	6.592%
38	12.992	1852	1854	1857	rVB	49704	41147	2.29%	0.158%
39	13.057	1863	1865	1868	rVB2	49378	41043	2.29%	0.157%
40	13.098	1869	1872	1874	rBV2	42574	43014	2.40%	0.165%
41	13.715	1974	1977	1982	rVB3	195558	222488	12.40%	0.853%
42	13.857	1996	2001	2004	rBV	1524324	1634282	91.12%	6.265%
43	14.039	2030	2032	2036	rVB3	75929	65091	3.63%	0.250%
44	14.339	2080	2083	2087	rBV2	207879	258786	14.43%	0.992%
45	14.633	2130	2133	2141	rBV	175730	269878	15.05%	1.035%
46	14.704	2142	2145	2154	rVB	204364	290037	16.17%	1.112%
47	14.862	2169	2172	2179	rBV	181396	348511	19.43%	1.336%
48	14.951	2183	2187	2196	rVB	624353	797049	44.44%	3.056%
49	15.204	2227	2230	2235	rVB	141669	152184	8.48%	0.583%
50	15.262	2236	2240	2244	rBV	1010884	1289631	71.90%	4.944%
51	15.709	2311	2316	2321	rBV	846428	1148025	64.01%	4.401%

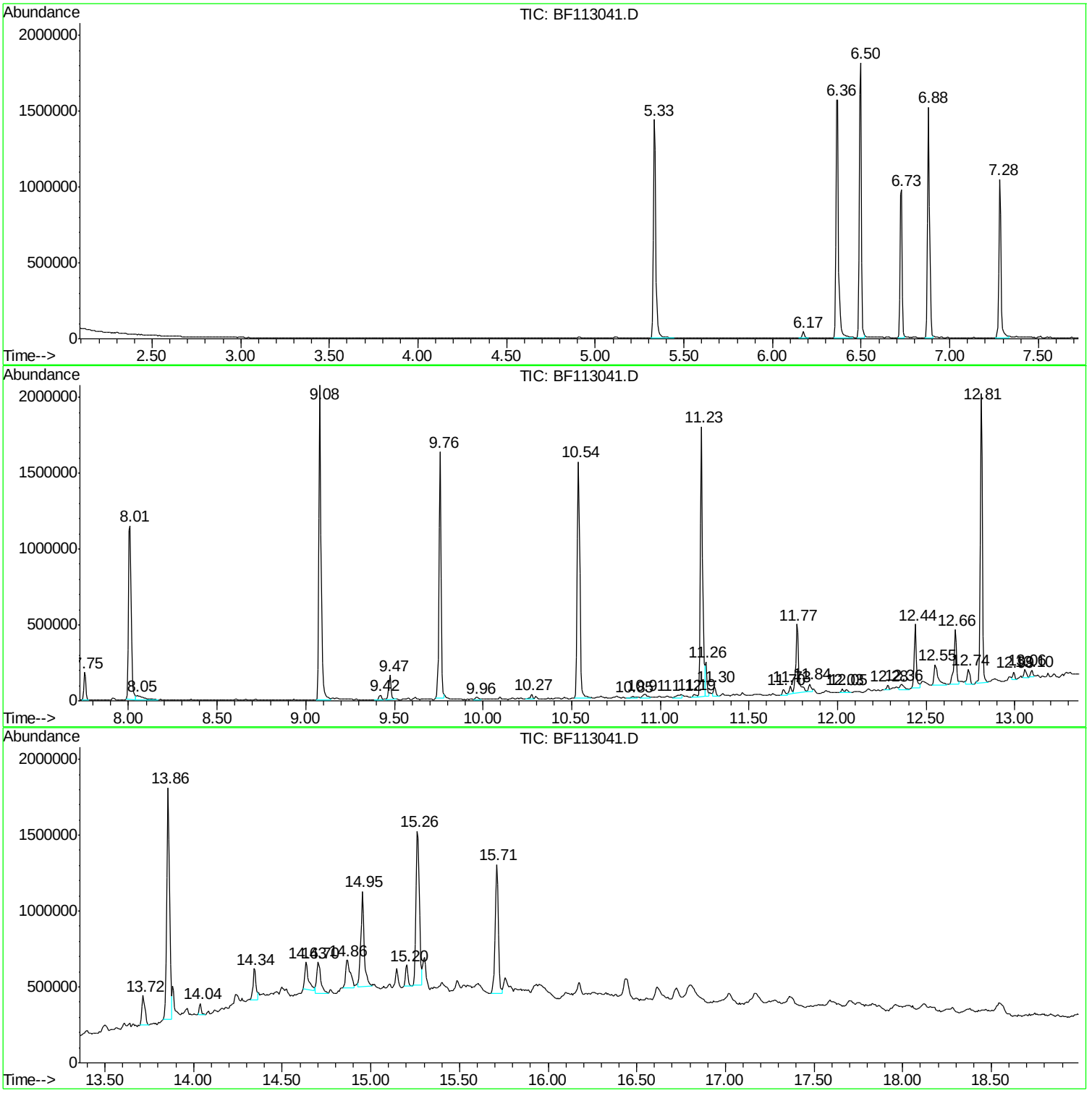
Sum of corrected areas: 26084990

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031319\
Data File : BF113042.D
Acq On : 13 Mar 2019 21:44
Operator : JU/SJ
Sample : K1870-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031319\
Data File : BF113042.D
Acq On : 13 Mar 2019 21:44
Operator : JU/SJ
Sample : K1870-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

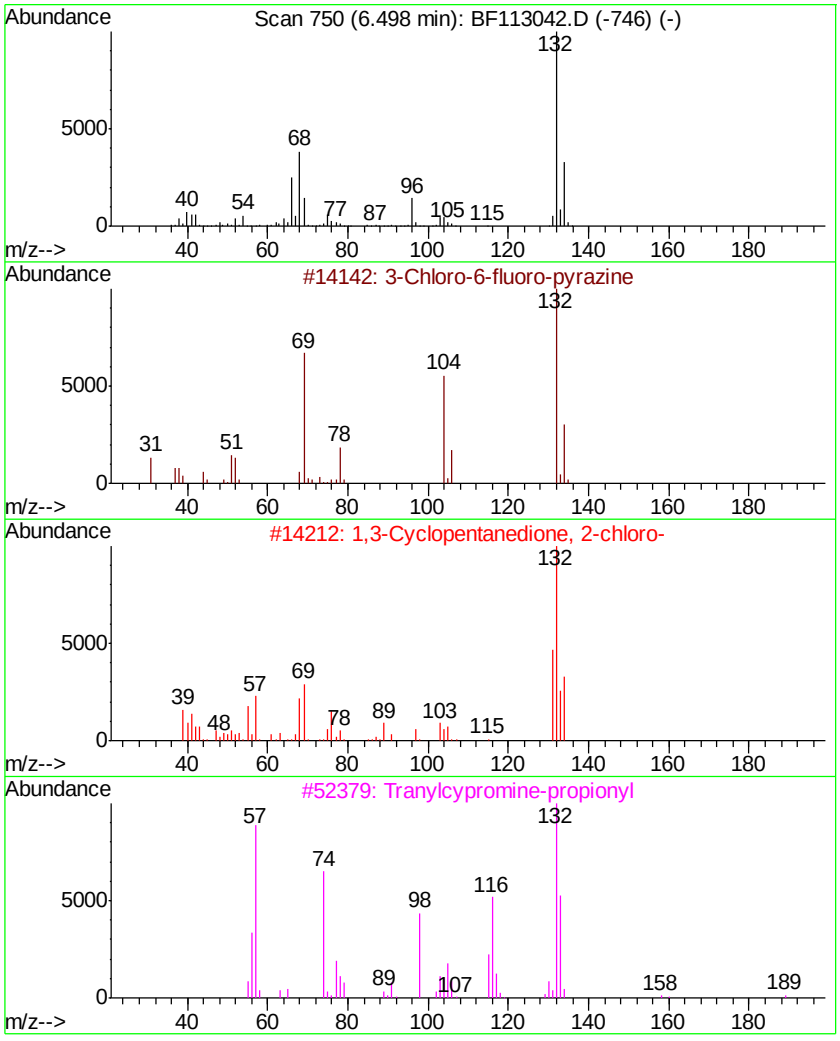
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

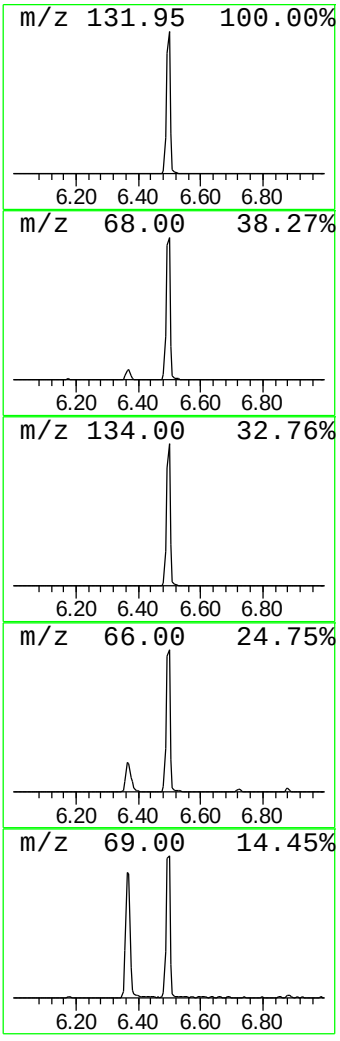
****

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	36.40 ng	1598120	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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031319\
Data File : BF113042.D
Acq On : 13 Mar 2019 21:44
Operator : JU/SJ
Sample : K1870-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1

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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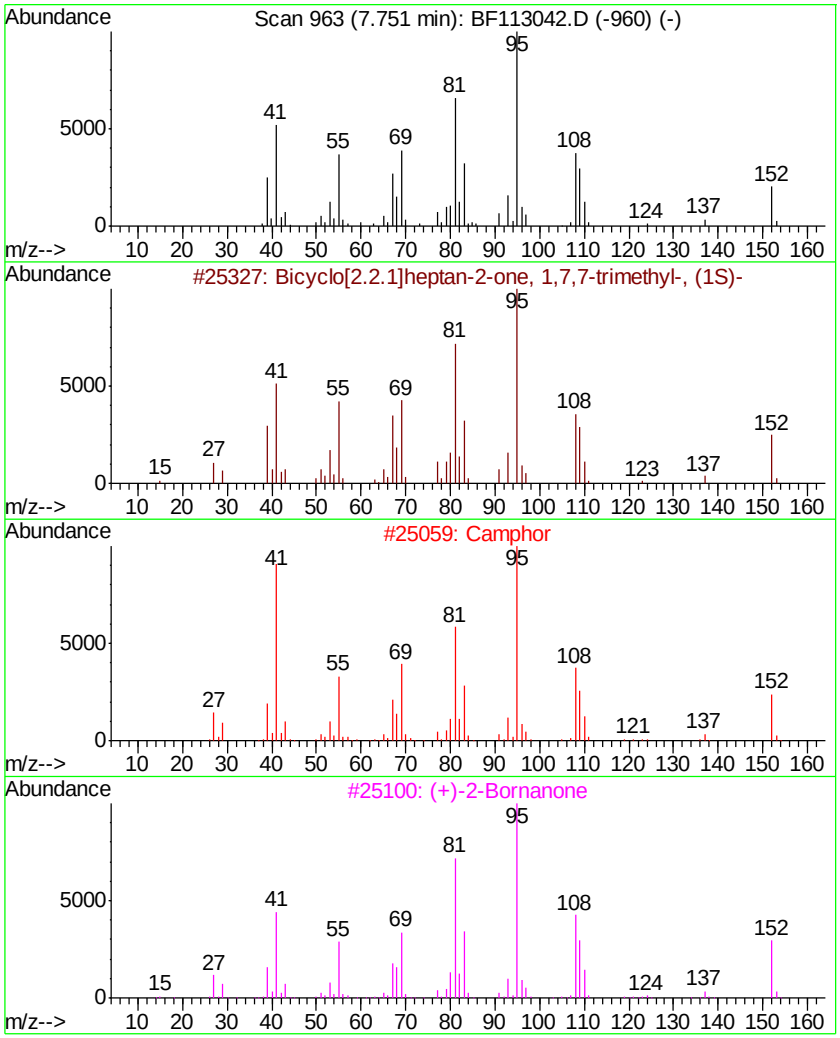
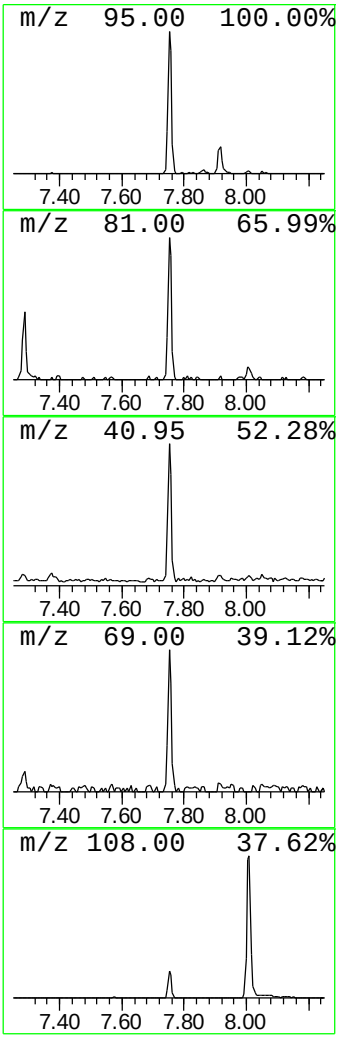
Peak Number 3 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.75	2.78 ng	156915	Naphthalene-d8	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	97
2	Camphor	152	C10H16O	000076-22-2	97
3	(+)-2-Bornanone	152	C10H16O	000464-49-3	96
4	5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	58
5	Bicyclo[3.1.0]hexan-2-one, 4-met...	152	C10H16O	002506-61-8	46





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031319\
Data File : BF113042.D
Acq On : 13 Mar 2019 21:44
Operator : JU/SJ
Sample : K1870-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1

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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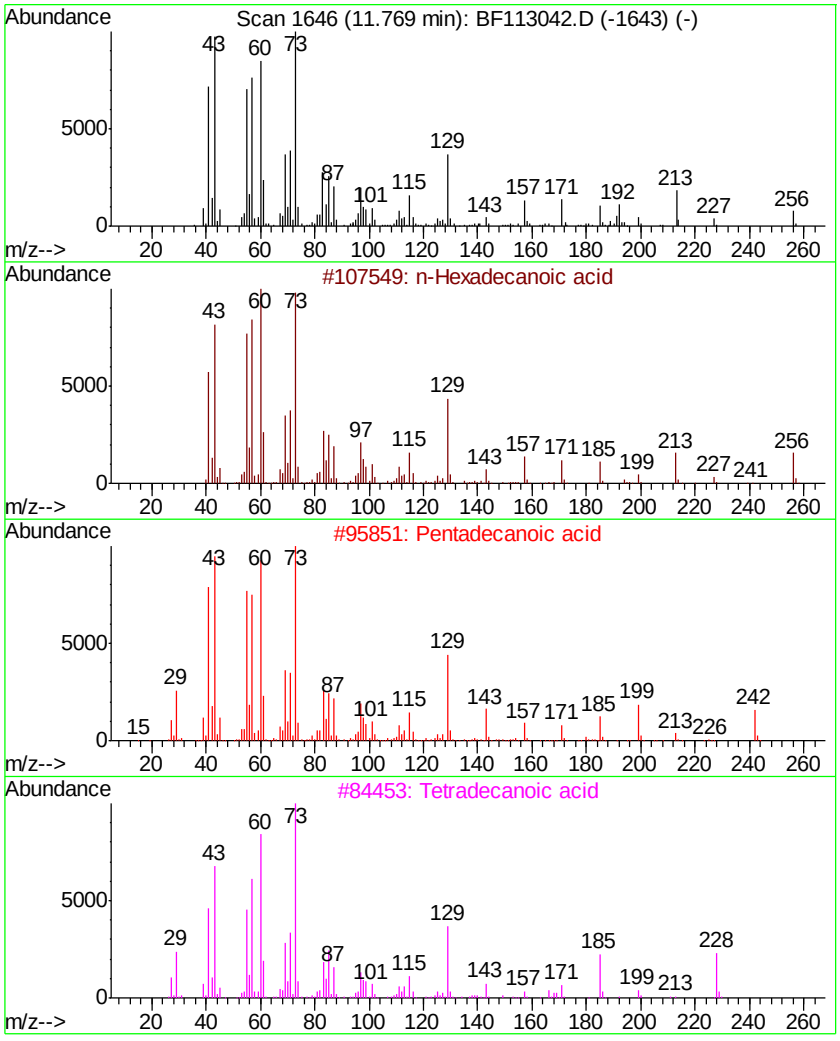
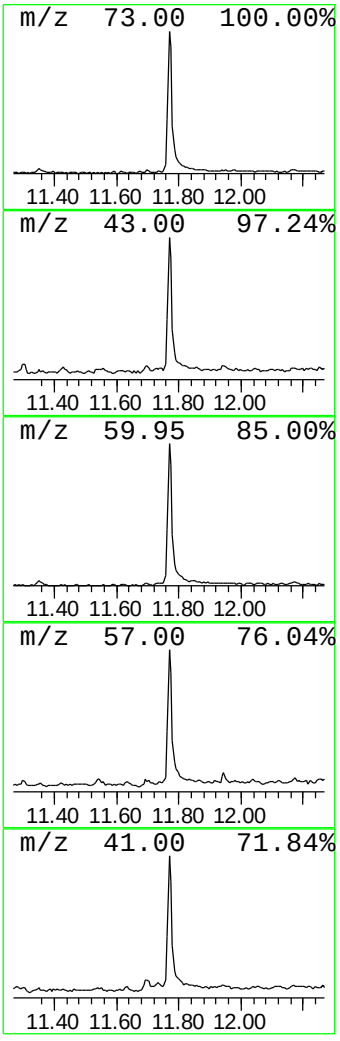
Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	6.49 ng	518442	Phenanthrene-d10	11.23

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	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	86
5	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	18





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031319\
Data File : BF113042.D
Acq On : 13 Mar 2019 21:44
Operator : JU/SJ
Sample : K1870-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

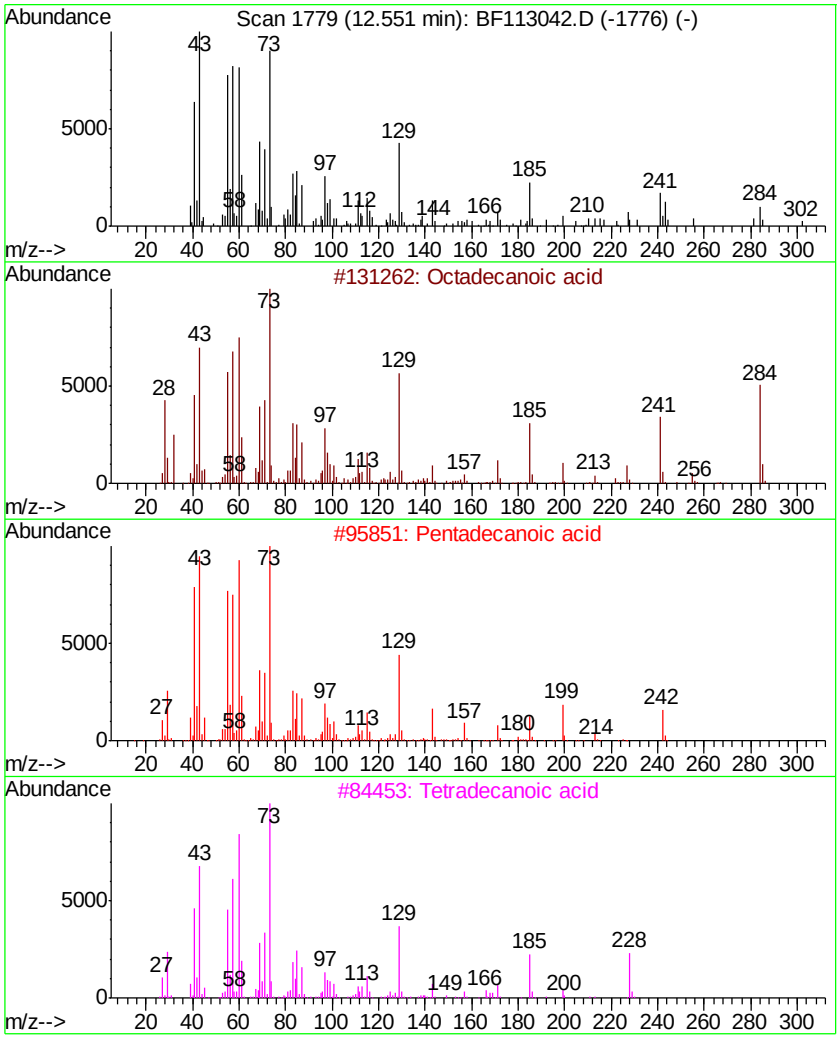
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

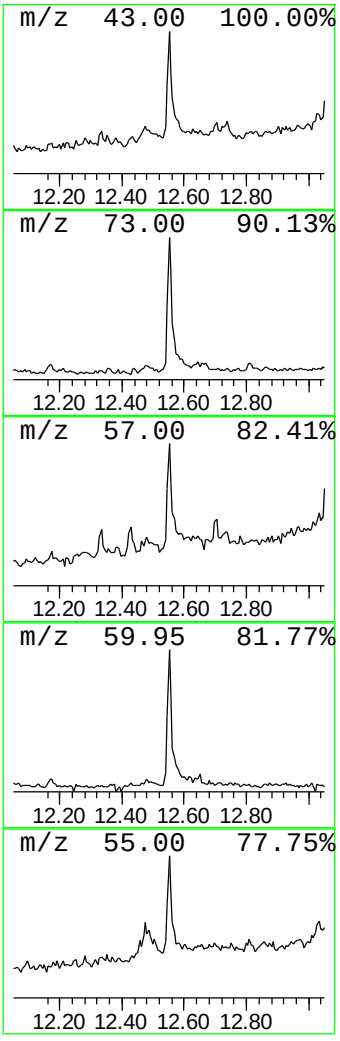
****

Peak Number 5 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.55	2.46 ng	201153	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
5	Tridecanoic acid	214	C13H26O2	000638-53-9	80





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031319\
Data File : BF113042.D
Acq On : 13 Mar 2019 21:44
Operator : JU/SJ
Sample : K1870-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1

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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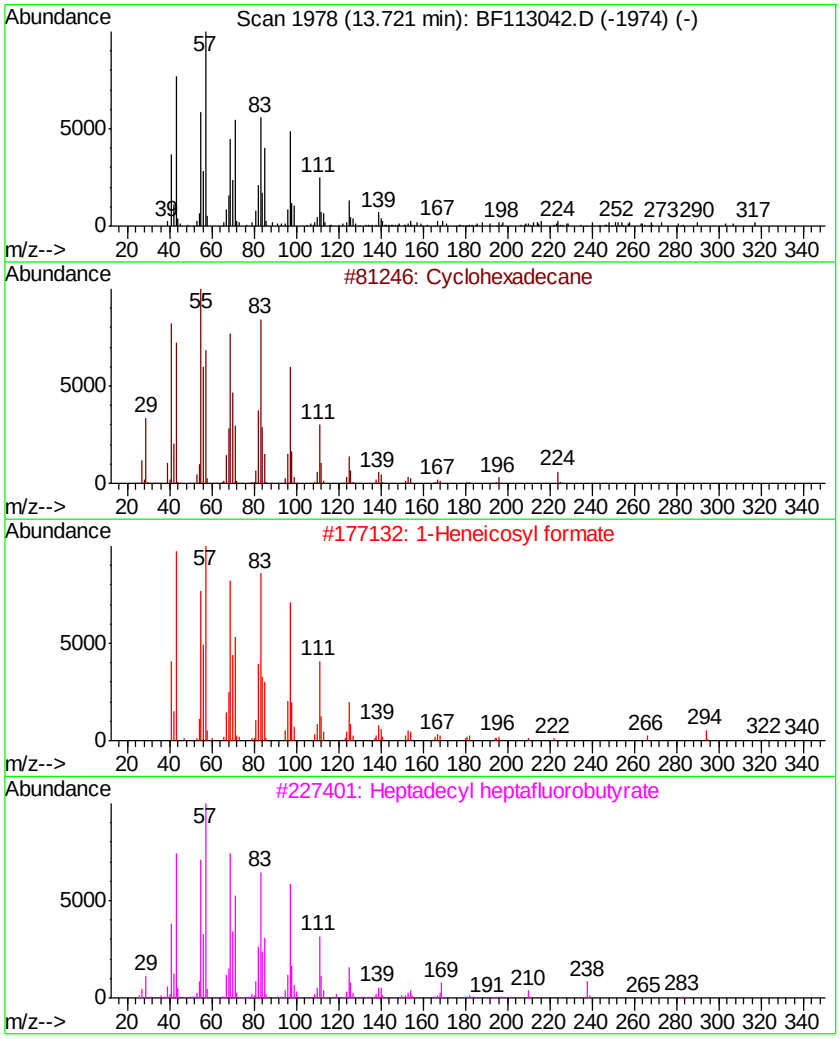
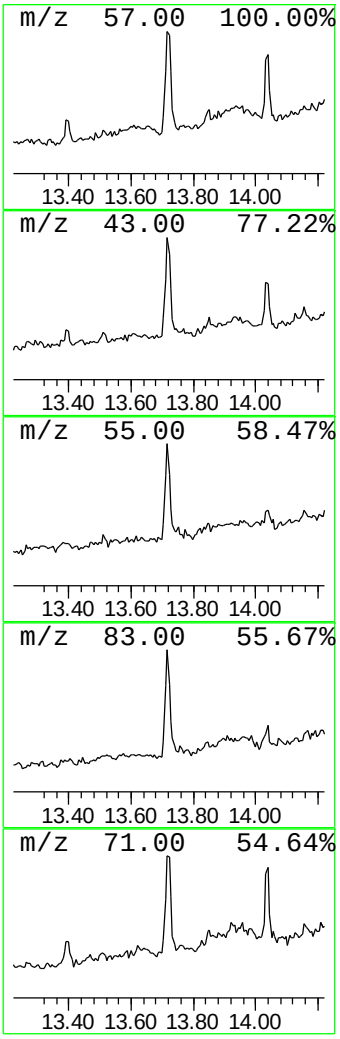
Peak Number 6 Cyclohexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	2.72 ng	222488	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	95
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031319\
Data File : BF113042.D
Acq On : 13 Mar 2019 21:44
Operator : JU/SJ
Sample : K1870-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1

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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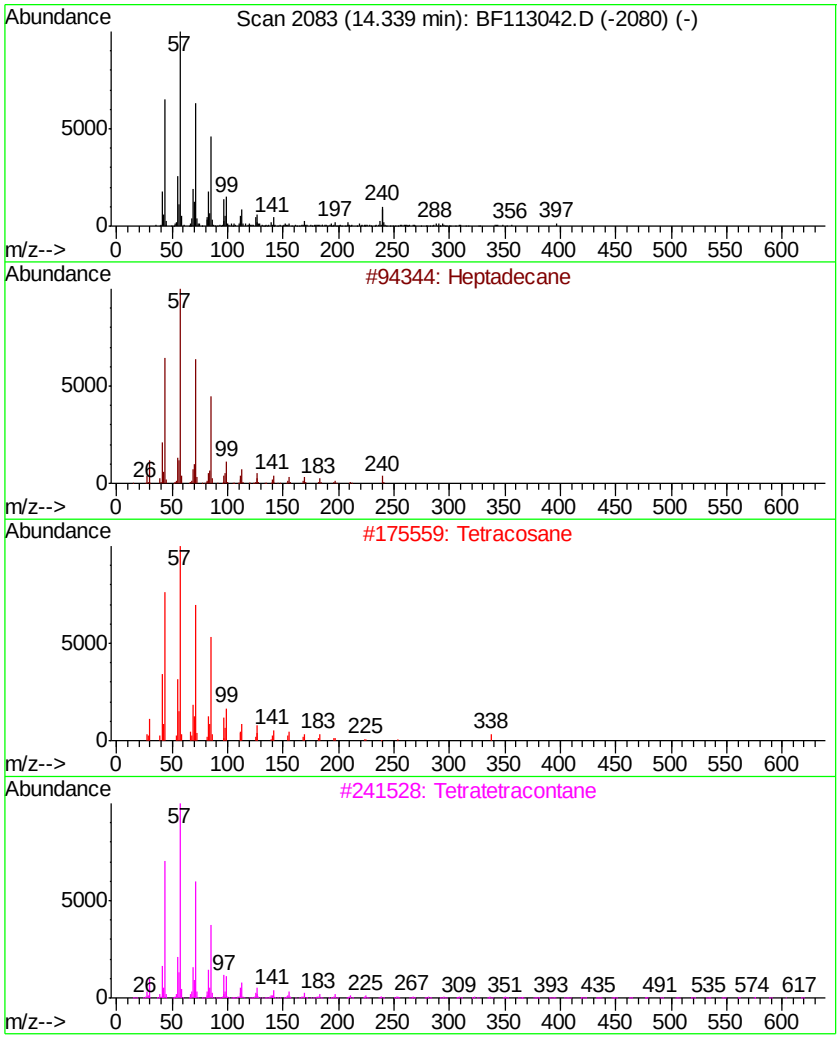
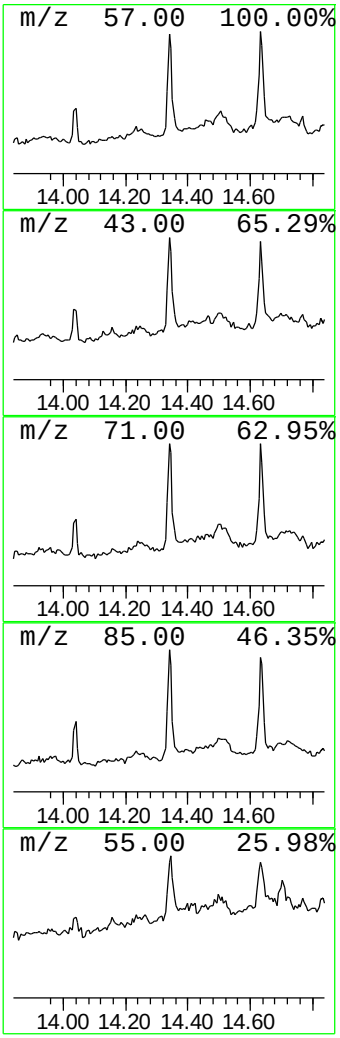
Peak Number 7 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	3.17 ng	258786	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	93
2	Tetracosane	338	C24H50	000646-31-1	87
3	Tetratetracontane	619	C44H90	007098-22-8	87
4	Heptacosane	380	C27H56	000593-49-7	87
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	83





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031319\
Data File : BF113042.D
Acq On : 13 Mar 2019 21:44
Operator : JU/SJ
Sample : K1870-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1

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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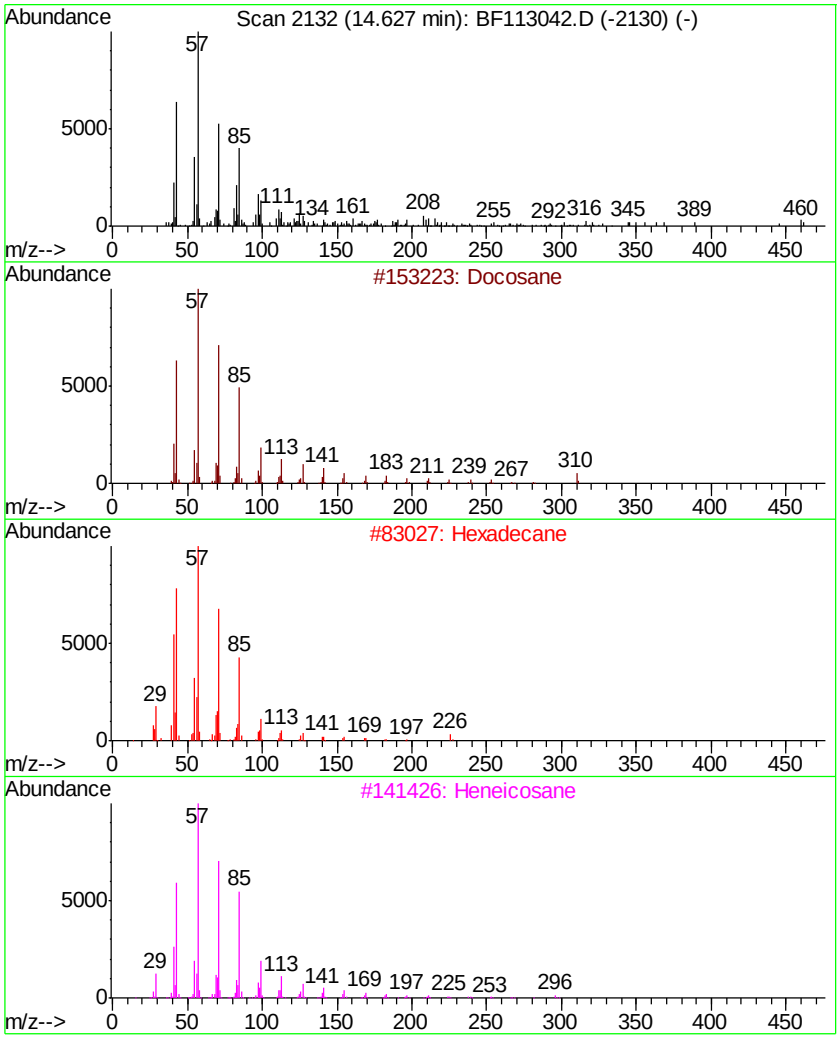
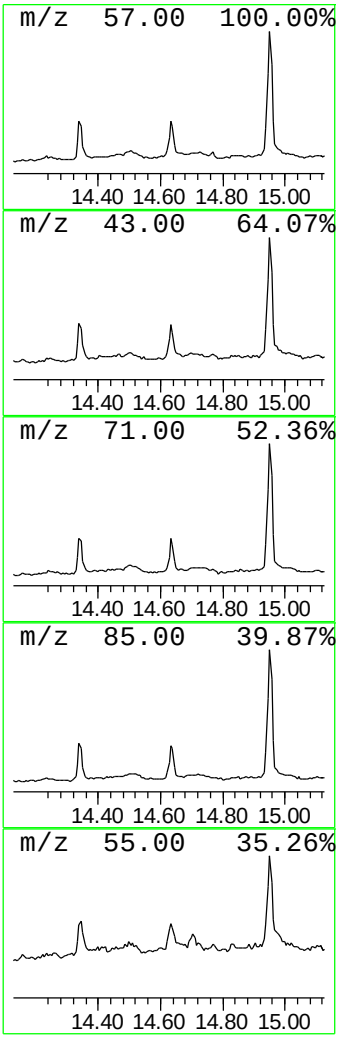
Peak Number 8 Docosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	4.19 ng	269878	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	93
2	Hexadecane	226	C16H34	000544-76-3	86
3	Heneicosane	296	C21H44	000629-94-7	86
4	Heptadecane	240	C17H36	000629-78-7	86
5	Octacosane	394	C28H58	000630-02-4	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031319\
Data File : BF113042.D
Acq On : 13 Mar 2019 21:44
Operator : JU/SJ
Sample : K1870-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1

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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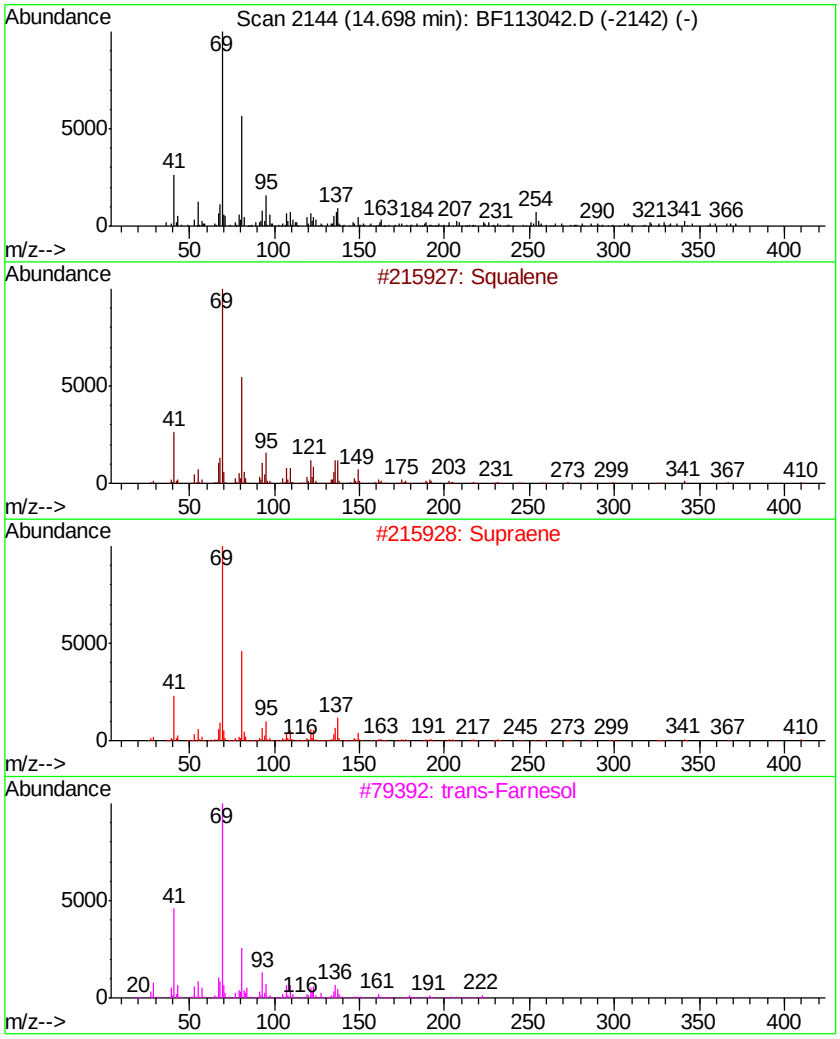
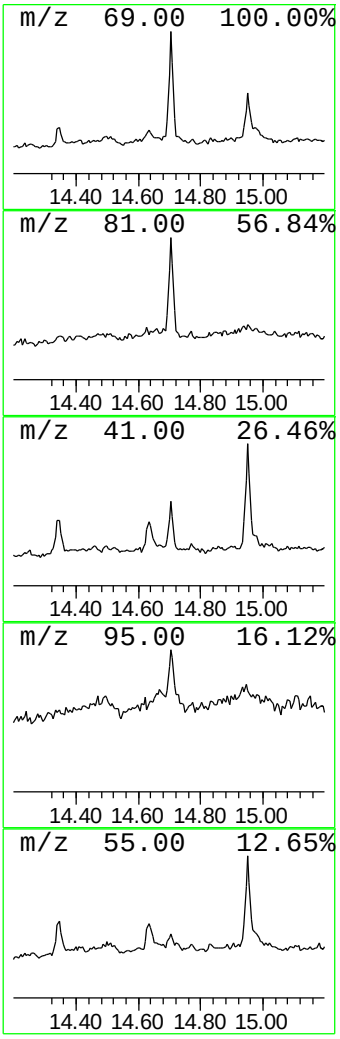
Peak Number 9 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	4.50 ng	290037	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	83
2	Supraene	410	C30H50	007683-64-9	81
3	trans-Farnesol	222	C15H26O	000106-28-5	70
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64





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Acq On : 13 Mar 2019 21:44
Operator : JU/SJ
Sample : K1870-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1

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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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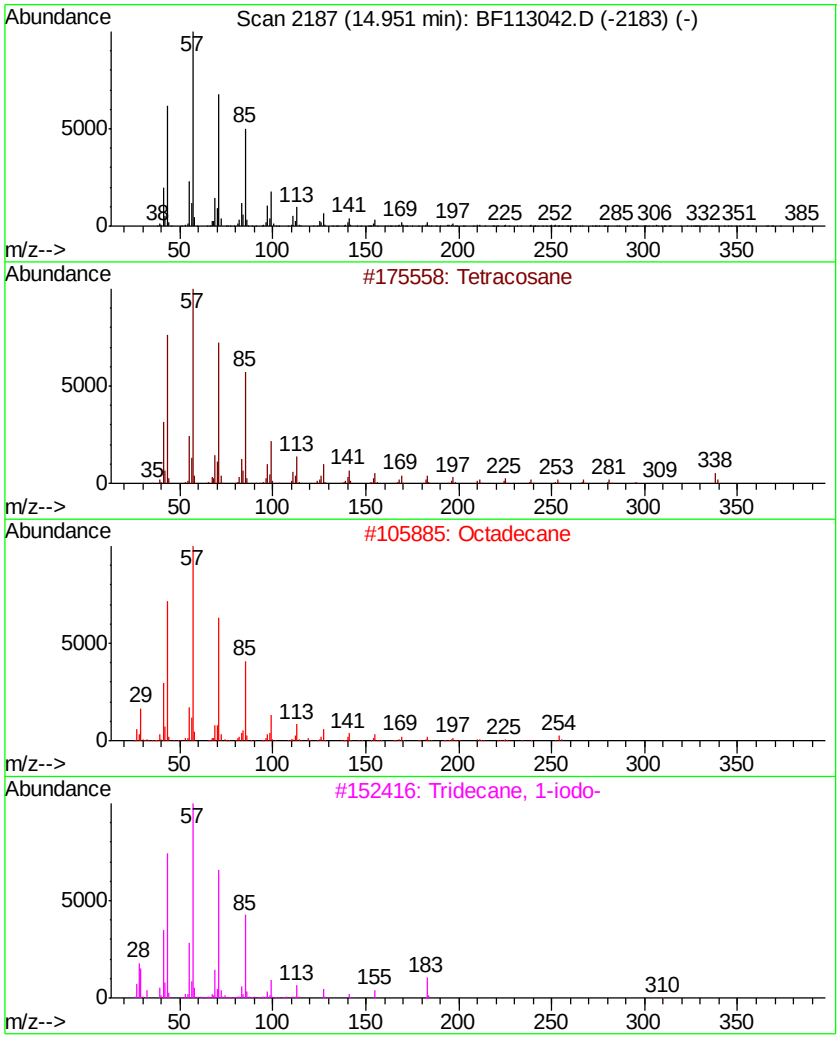
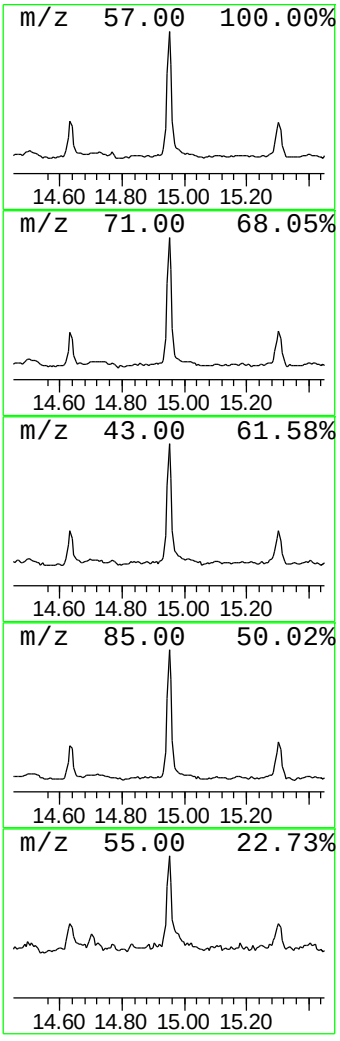
Peak Number 10 Tetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	12.36 ng	797049	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	97
2	Octadecane	254	C18H38	000593-45-3	93
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	93
4	Heneicosane	296	C21H44	000629-94-7	91
5	Hexacosane	366	C26H54	000630-01-3	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031319\
Data File : BF113042.D
Acq On : 13 Mar 2019 21:44
Operator : JU/SJ
Sample : K1870-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1

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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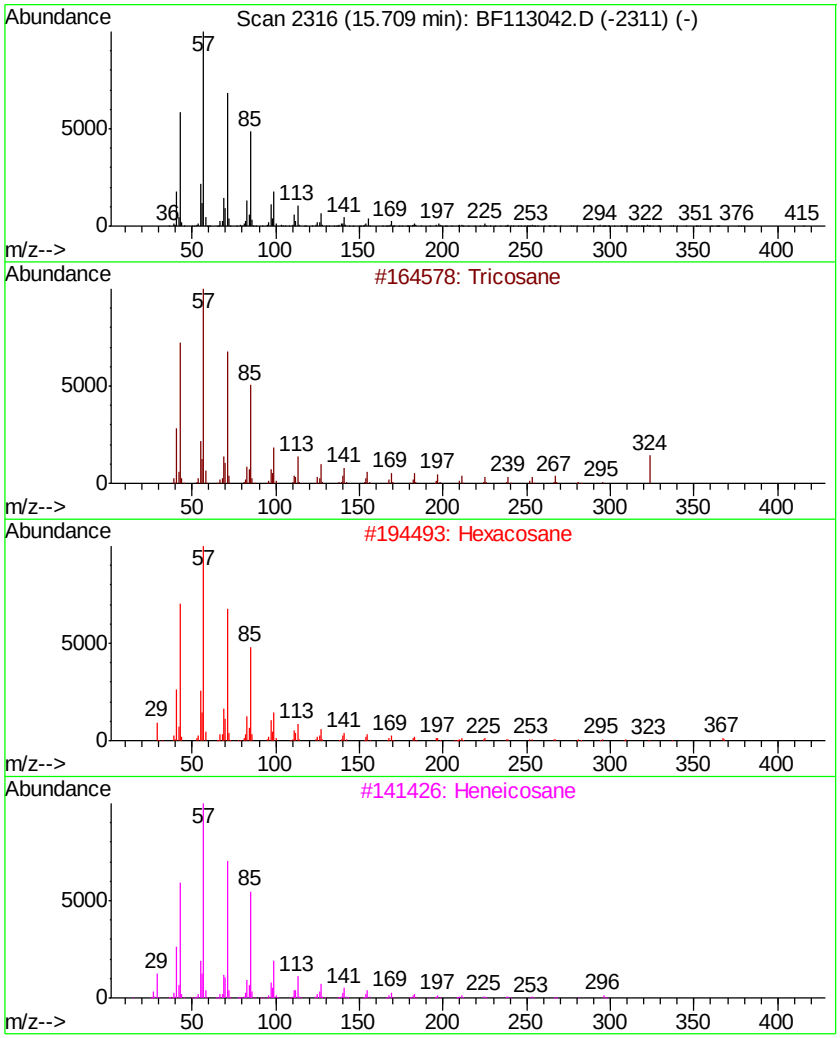
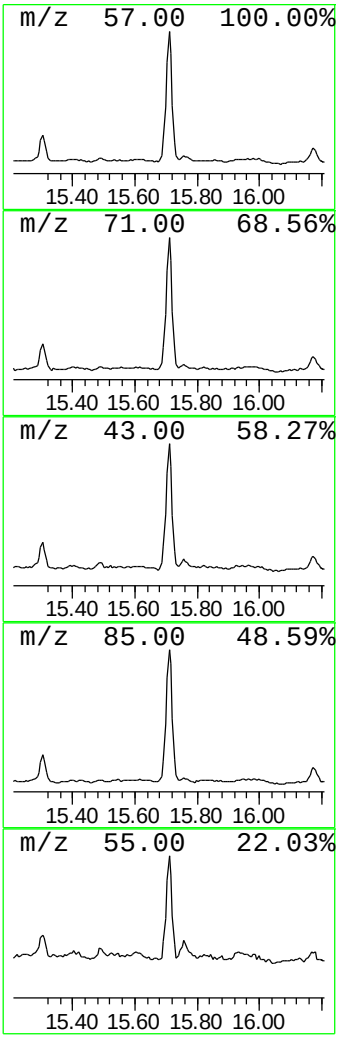
Peak Number 11 Tricosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	17.80 ng	1148030	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	93
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	91
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031319\
Data File : BF113042.D
Acq On : 13 Mar 2019 21:44
Operator : JU/SJ
Sample : K1870-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1

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	36.4	ng	1598120	1	6.73	878132	20.0
Bicyclo[2.2.1]hep...	7.75	2.8	ng	156915	2	8.01	1127810	20.0
n-Hexadecanoic acid	11.77	6.5	ng	518442	4	11.23	1598860	20.0
Octadecanoic acid	12.55	2.5	ng	201153	5	13.86	1634280	20.0
Cyclohexadecane	13.72	2.7	ng	222488	5	13.86	1634280	20.0
Heptadecane	14.34	3.2	ng	258786	5	13.86	1634280	20.0
Docosane	14.63	4.2	ng	269878	6	15.26	1289630	20.0
Squalene	14.70	4.5	ng	290037	6	15.26	1289630	20.0
Tetracosane	14.95	12.4	ng	797049	6	15.26	1289630	20.0
Tricosane	15.71	17.8	ng	1148030	6	15.26	1289630	20.0