LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070819\
Data File : BF115428.D
Acq On : 9 Jul 2019 1:37
Operator : HP/JU
Sample : K3681-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PILEA-07-01-19

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-BF070519.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	2.199	12	19	26	rVB	1319370	1758418	39.55%	4.125%
2	5.516	577	583	586	rBV	3674350	3636520	81.80%	8.532%
3	6.522	748	754	757	rBV	3626500	3907410	87.89%	9.167%
4	6.663	773	778	781	rBV	3983503	3981895	89.56%	9.342%
5	6.892	813	817	821	rVB	1433471	1132551	25.47%	2.657%
6	7.051	840	844	847	rBV	3625102	3112580	70.01%	7.303%
7	7.451	907	912	915	rBV	2762764	2527519	56.85%	5.930%
8	8.175	1031	1035	1038	rBV	1900187	1496416	33.66%	3.511%
9	9.251	1213	1218	1221	rBV	5143197	4445887	100.00%	10.431%
10	9.369	1235	1238	1241	rVB2	53587	53369	1.20%	0.125%
11	9.639	1280	1284	1287	rBV	570396	517391	11.64%	1.214%
12	9.910	1325	1330	1331	rBV	400934	395823	8.90%	0.929%
13	9.927	1331	1333	1337	rVB2	2054422	1636694	36.81%	3.840%
14	10.710	1462	1466	1470	rBV	2613253	2514437	56.56%	5.899%
15	11.410	1581	1585	1588	rBV	2049616	1689924	38.01%	3.965%
16	11.645	1619	1625	1633	rBV4	31569	67786	1.52%	0.159%
17	11.933	1671	1674	1678	rBV	299350	260826	5.87%	0.612%
18	12.616	1787	1790	1793	rBV	110836	99097	2.23%	0.232%
19	12.716	1804	1807	1815	rBV3	82318	102296	2.30%	0.240%
20	12.845	1826	1829	1832	rVB	80387	61405	1.38%	0.144%
21	12.992	1849	1854	1857	rBV	4174807	3786490	85.17%	8.884%
22	13.227	1887	1894	1898	rBV3	53748	72796	1.64%	0.171%
23	13.645	1959	1965	1969	rBV8	41652	101319	2.28%	0.238%
24	13.745	1979	1982	1986	rBV	548591	462704	10.41%	1.086%
25	13.898	2004	2008	2022	rVB	391883	592091	13.32%	1.389%
26	14.039	2027	2032	2035	rBV	1335898	1288964	28.99%	3.024%
27	14.062	2035	2036	2045	rVB	62049	57901	1.30%	0.136%
28	14.215	2058	2062	2067	rBV	58903	87549	1.97%	0.205%
29	14.515	2111	2113	2115	rBV	86263	82230	1.85%	0.193%
30	14.539	2115	2117	2127	rVB3	92678	162367	3.65%	0.381%
31	14.827	2162	2166	2170	rVB	117854	126588	2.85%	0.297%
32	14.904	2176	2179	2185	rVB	115140	117021	2.63%	0.275%
33	14.968	2187	2190	2197	rBV4	82669	116776	2.63%	0.274%
34	15.080	2205	2209	2212	rBV	48371	69327	1.56%	0.163%

LSC Area Percent Report

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Operator : HP/JU
Sample : K3681-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PILEA-07-01-19

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-BF070519.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.168	2220	2224	2227	rBV	141620	163229	3.67%	0.383%
36	15.209	2227	2231	2235	rVV2	58962	98329	2.21%	0.231%
37	15.509	2277	2282	2286	rBV	942467	1213552	27.30%	2.847%
38	15.557	2286	2290	2298	rVB	117124	170685	3.84%	0.400%
39	15.756	2321	2324	2328	rVB3	42849	57387	1.29%	0.135%
40	15.998	2361	2365	2370	rVB	123411	176881	3.98%	0.415%
41	16.062	2372	2376	2385	rVV4	61761	162293	3.65%	0.381%
42	16.509	2449	2452	2457	rVB	42726	58673	1.32%	0.138%

Sum of corrected areas: 42623396

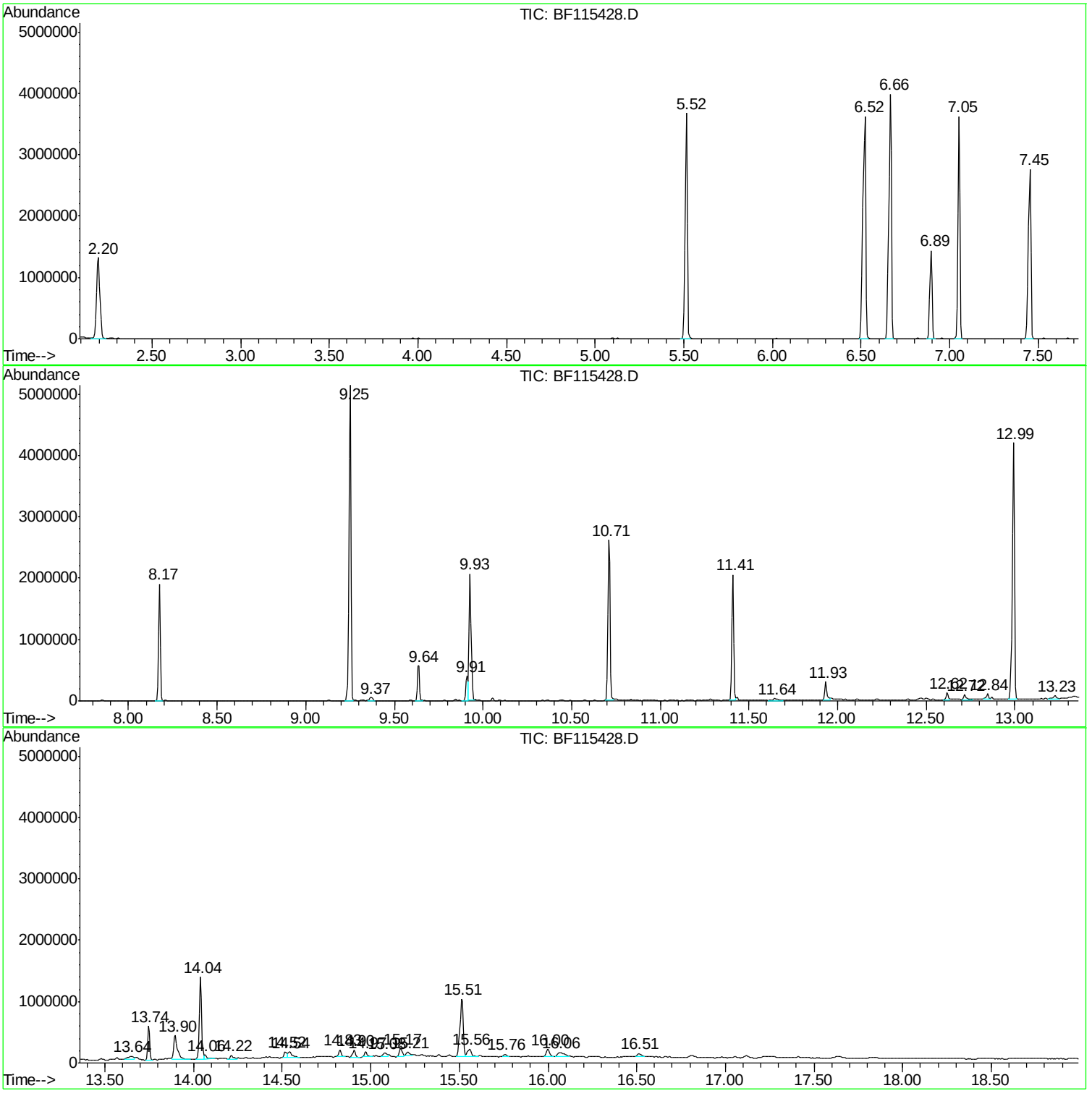
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070819\
Data File : BF115428.D
Acq On : 9 Jul 2019 1:37
Operator : HP/JU
Sample : K3681-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PILEA-07-01-19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.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\BF070819\
Data File : BF115428.D
Acq On : 9 Jul 2019 1:37
Operator : HP/JU
Sample : K3681-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PILEA-07-01-19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

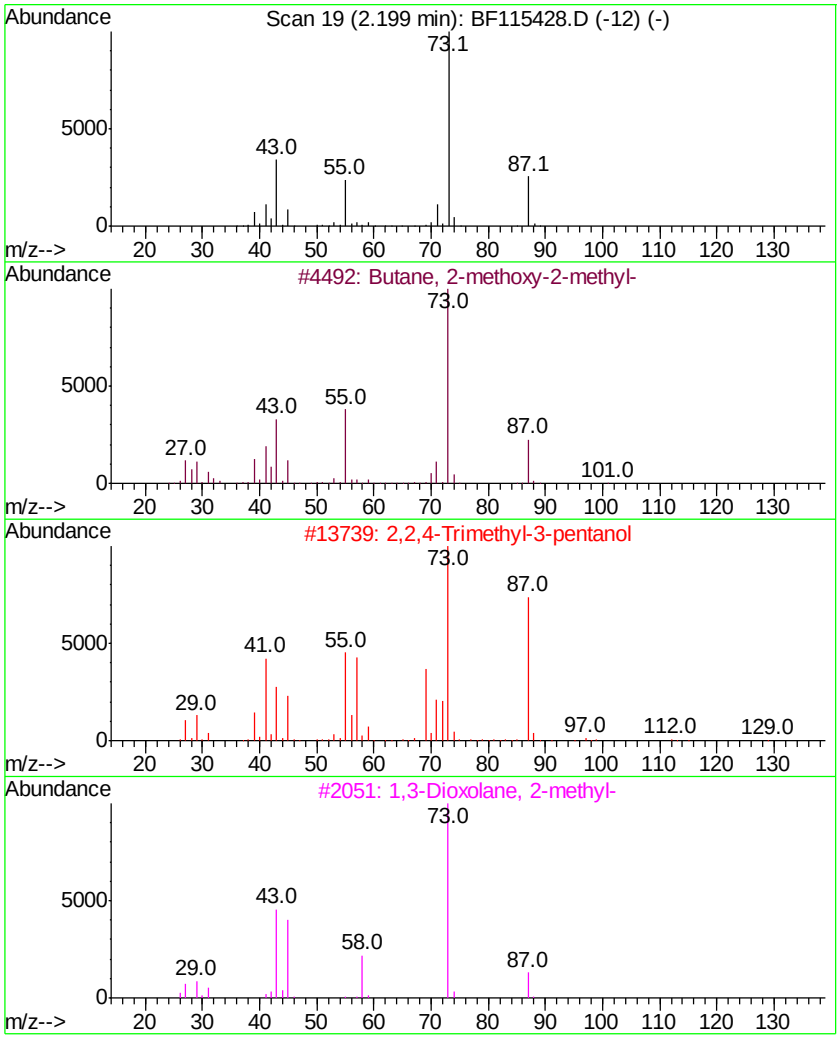
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

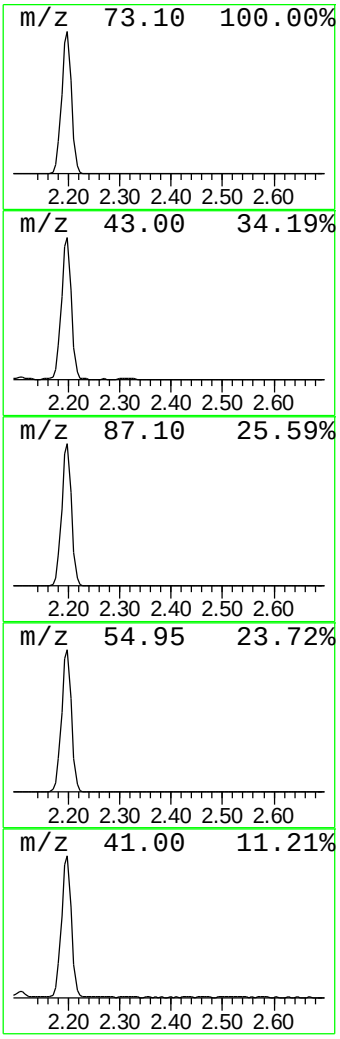
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	31.05 ng	1758420	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	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





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Data File : BF115428.D
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Operator : HP/JU
Sample : K3681-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PILEA-07-01-19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

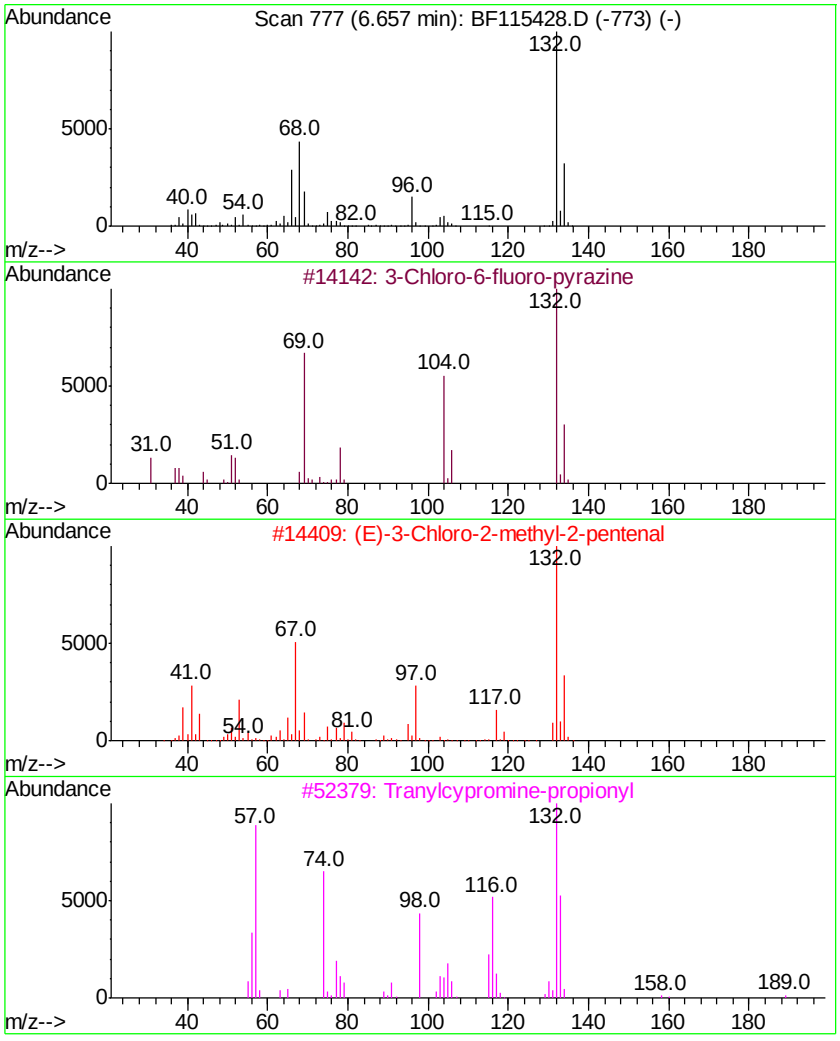
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

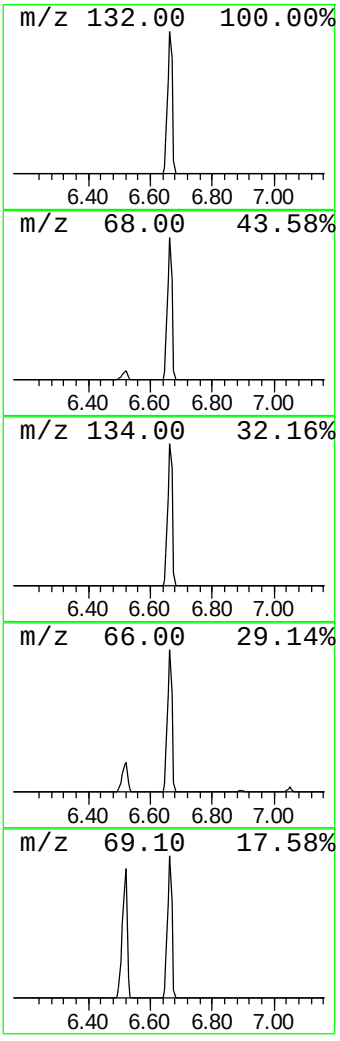
****

Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	70.32 ng	3981900	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	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Data File : BF115428.D
Acq On : 9 Jul 2019 1:37
Operator : HP/JU
Sample : K3681-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PILEA-07-01-19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

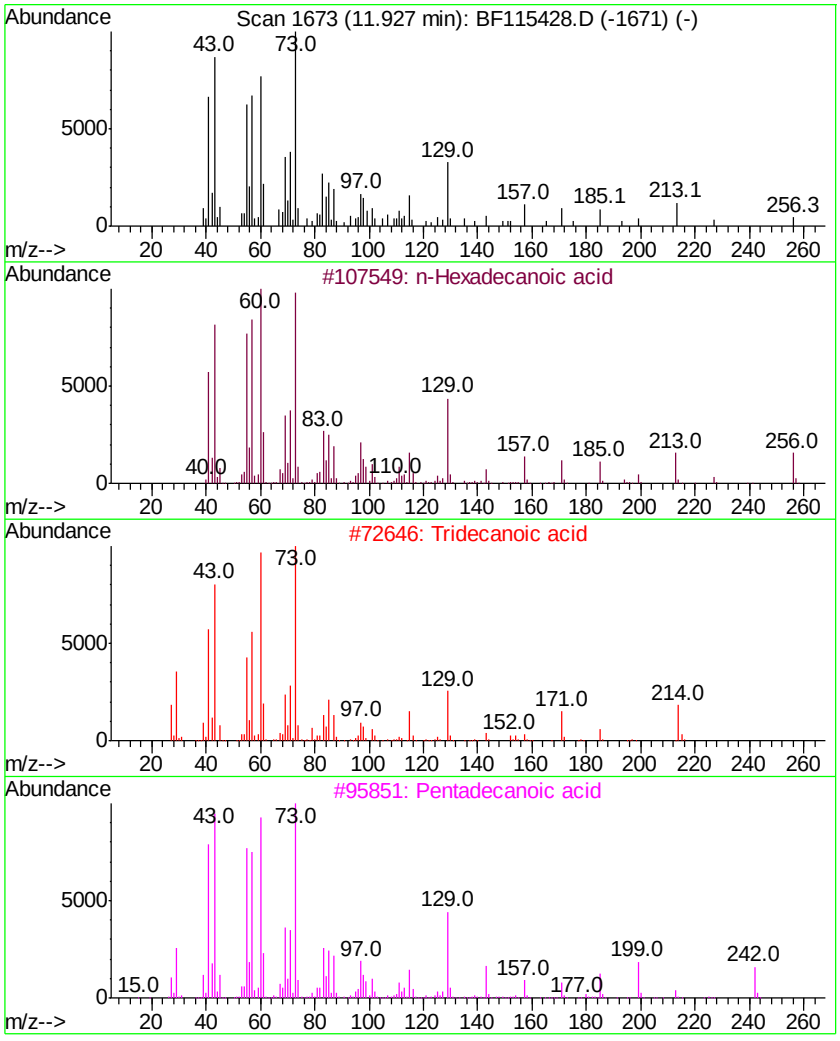
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

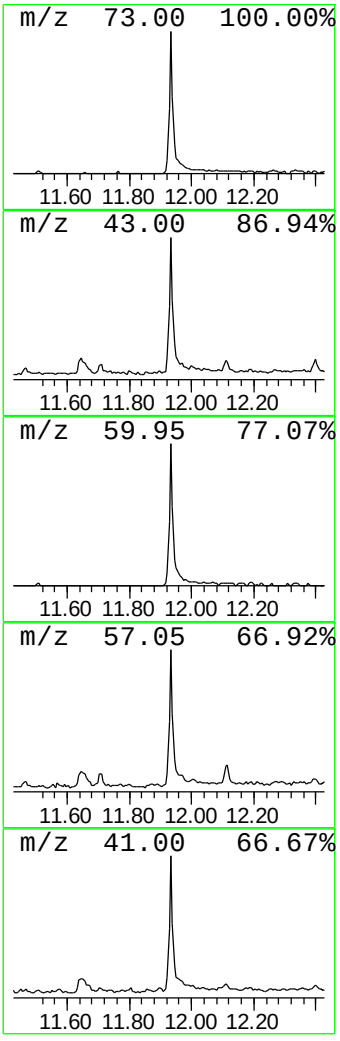
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	3.09 ng	260826	Phenanthrene-d10	11.41

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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





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Data File : BF115428.D
Acq On : 9 Jul 2019 1:37
Operator : HP/JU
Sample : K3681-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PILEA-07-01-19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.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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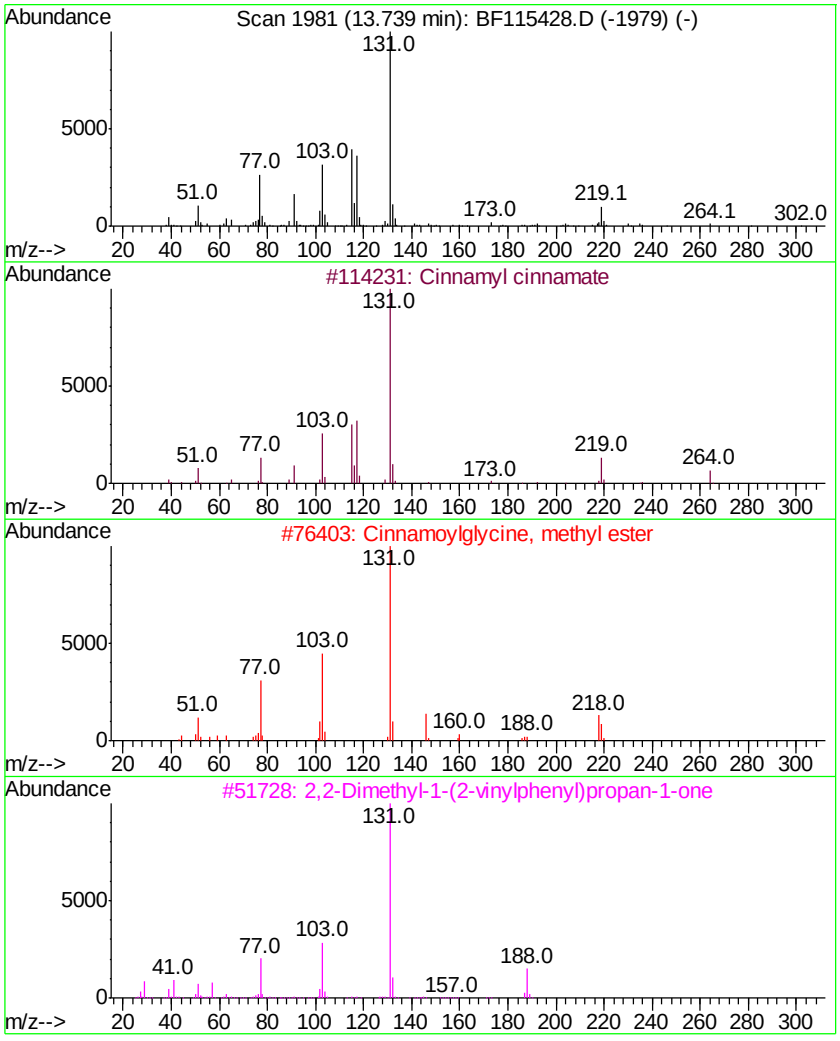
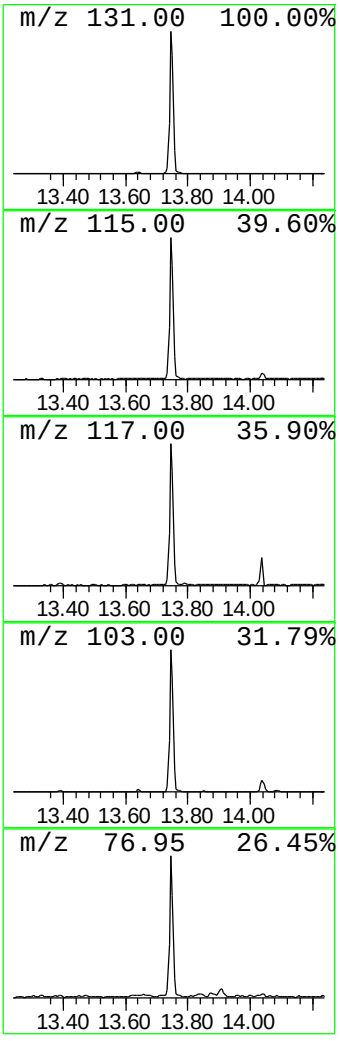
Peak Number 5 Cinnamyl cinnamate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	7.18 ng	462704	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	87
2	Cinnamoylglycine, methyl ester	219	C12H13NO3	040778-04-9	70
3	2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	52
4	2-Iodo-benzoic acid N'-(3-phenyl...	392	C16H13IN2O2	315672-62-9	50
5	trans-1-Cinnamoylimidazole	198	C12H10N2O	001138-15-4	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070819\
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Sample : K3681-01
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Instrument : BNA_F
ClientSampleId : PILEA-07-01-19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

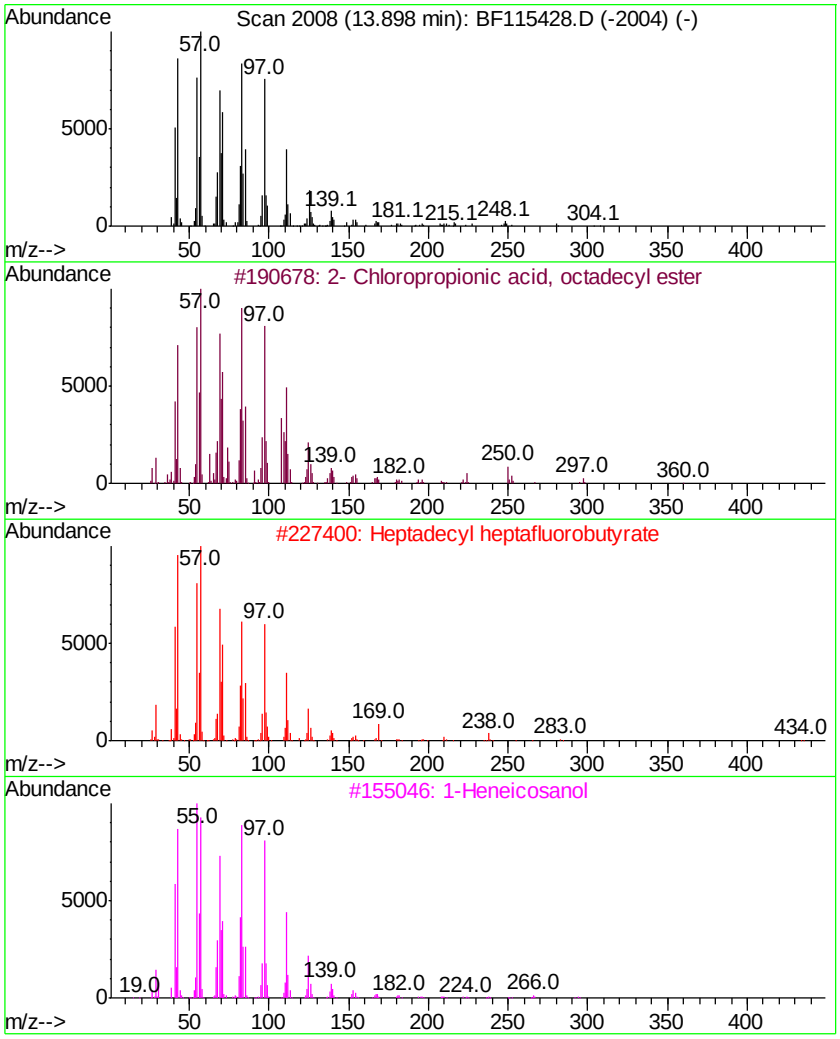
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

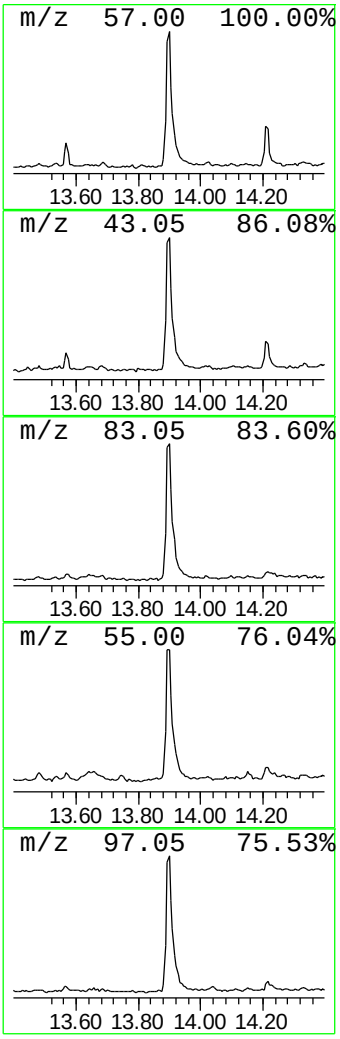
****

Peak Number 6 2- Chloropropionic acid, oc... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	9.19 ng	592091	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	93
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93





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Sample : K3681-01
Misc :
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Instrument : BNA_F
ClientSampleId : PILEA-07-01-19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.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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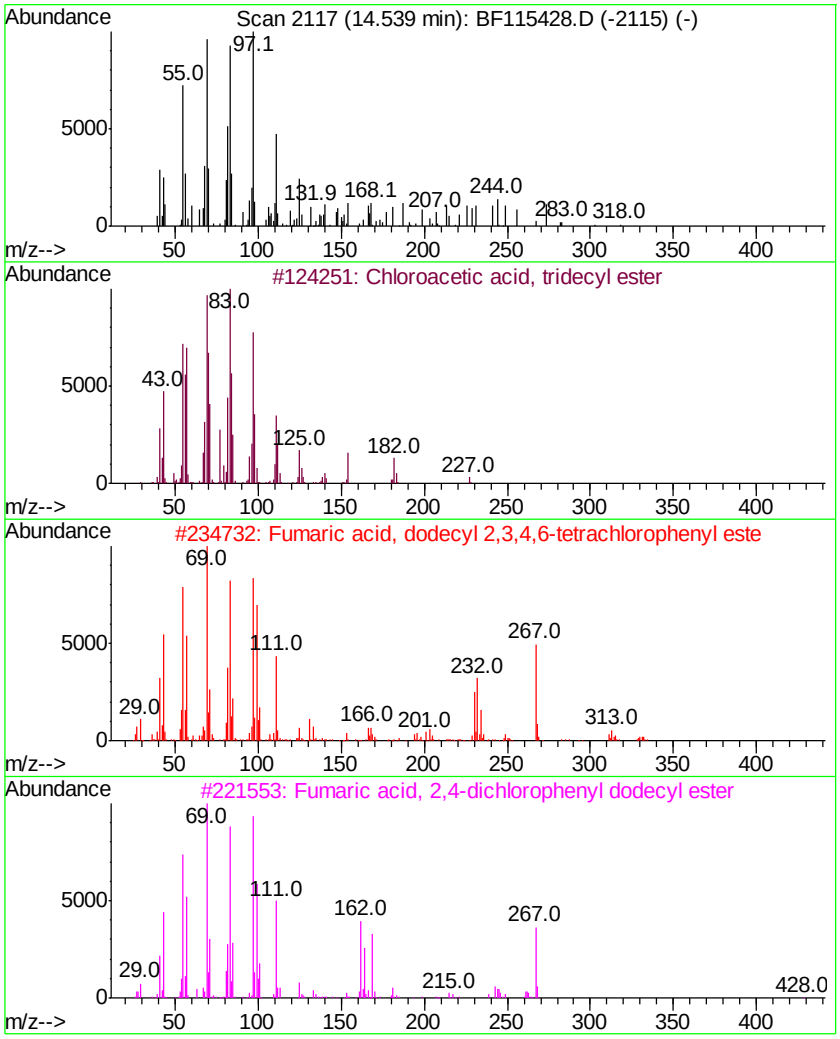
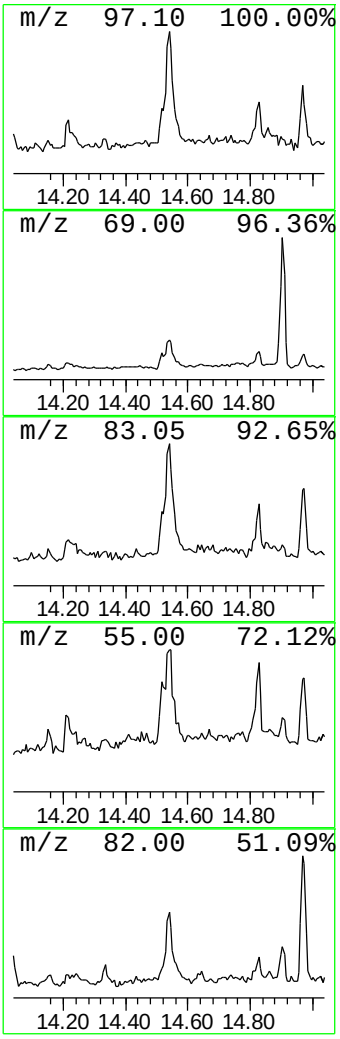
Peak Number 7 Chloroacetic acid, tridecyl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.54	2.52 ng	162367	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Chloroacetic acid, tridecyl ester	276	C15H29ClO2	018277-85-5	72
2	Fumaric acid, dodecyl 2,3,4,6-te...	496	C22H28Cl4O4	1000348-20-4	59
3	Fumaric acid, 2,4-dichlorophenyl...	428	C22H30Cl2O4	1000345-34-4	59
4	3-Octene, 2,2-dimethyl-	140	C10H20	086869-76-3	46
5	7-Tetradecanol	214	C14H30O	003981-79-1	43





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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PILEA-07-01-19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.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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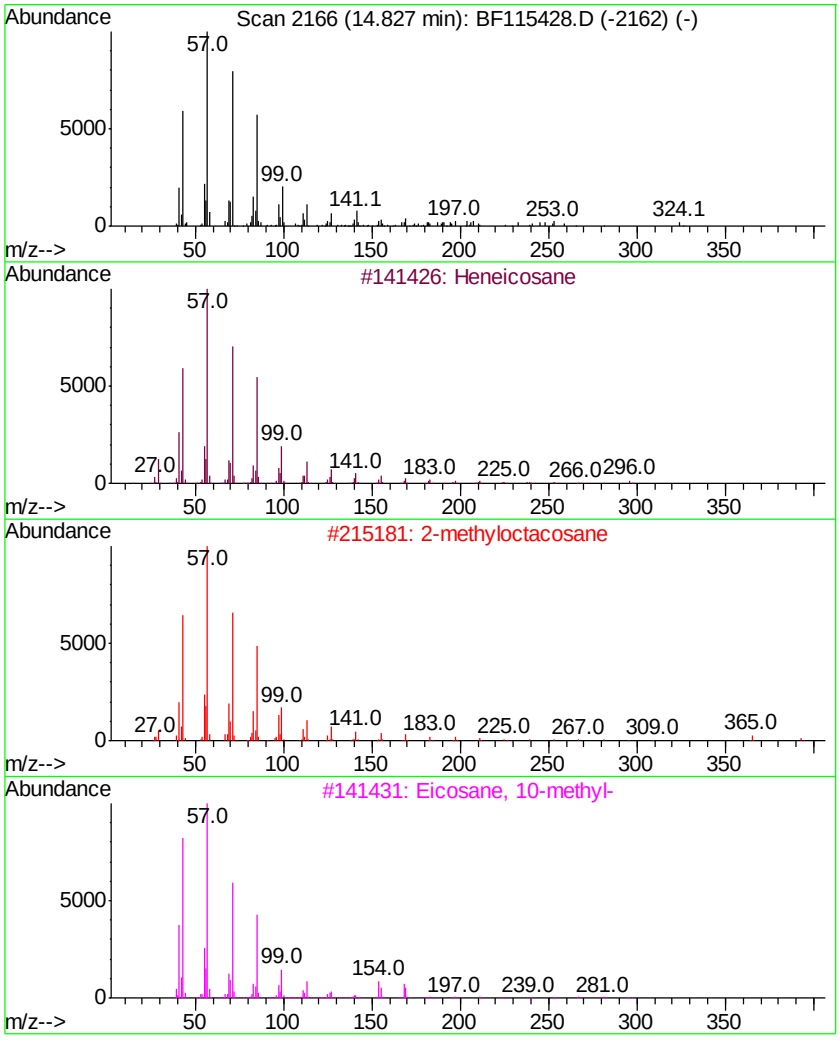
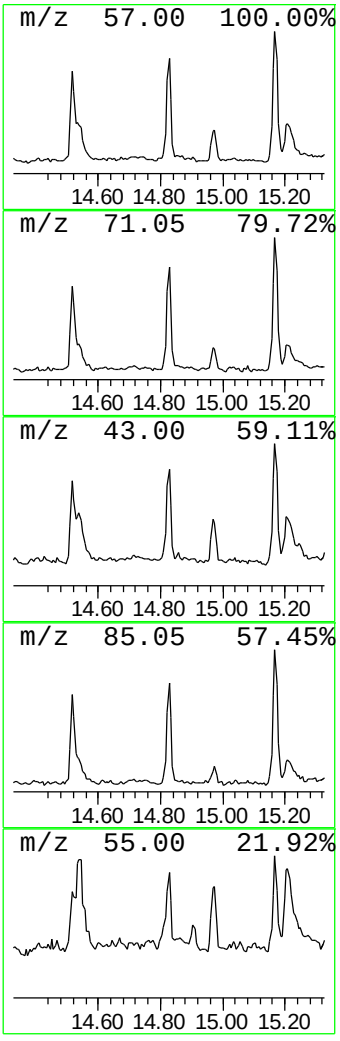
Peak Number 8 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	2.09 ng	126588	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
4	Pentacosane	352	C25H52	000629-99-2	90
5	Octacosane	394	C28H58	000630-02-4	90





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Data File : BF115428.D
Acq On : 9 Jul 2019 1:37
Operator : HP/JU
Sample : K3681-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PILEA-07-01-19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.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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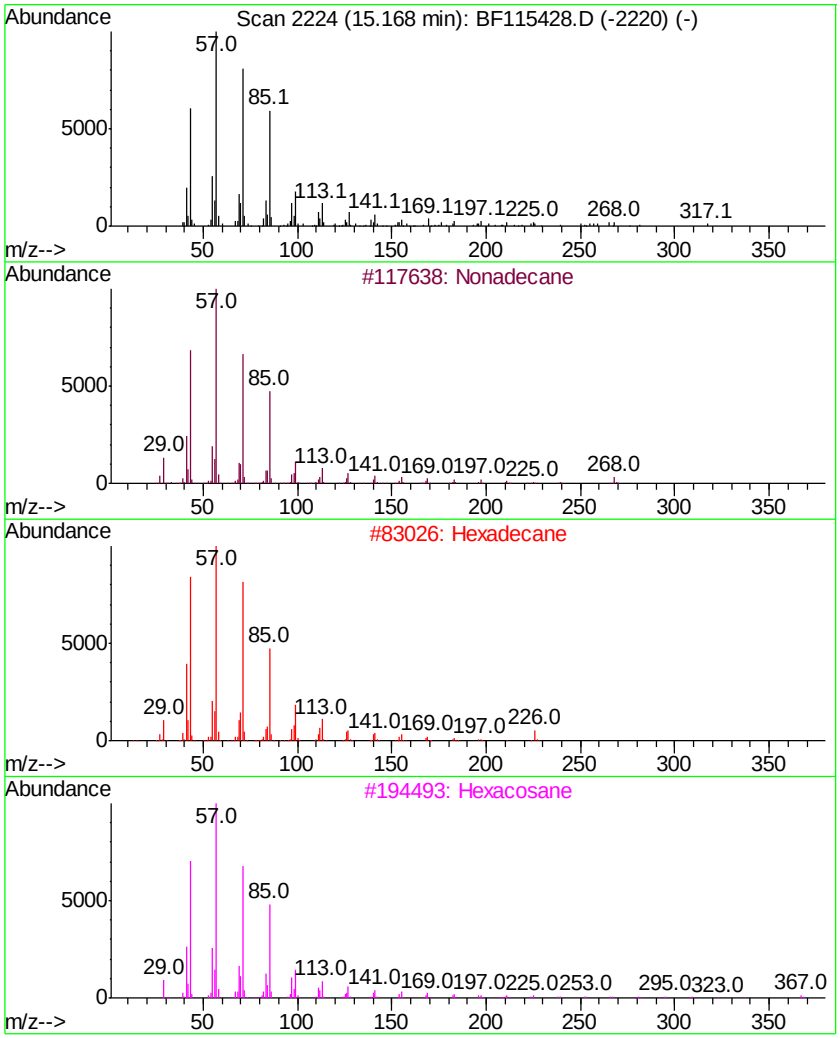
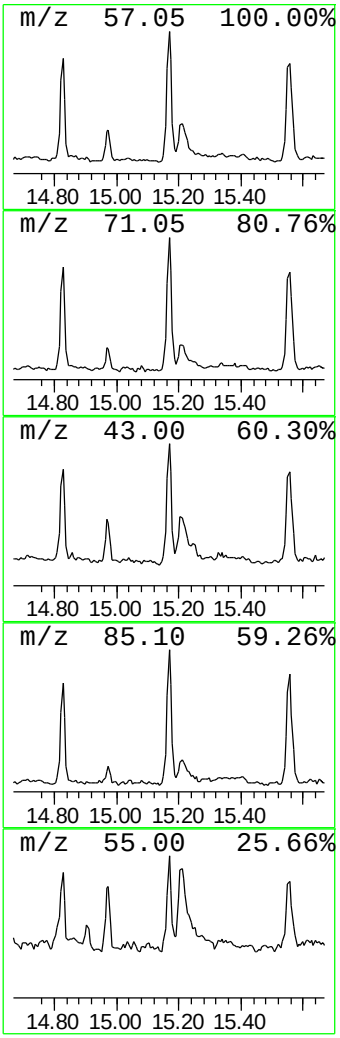
Peak Number 9 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	2.69 ng	163229	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	93
2	Hexadecane	226	C16H34	000544-76-3	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Heneicosane	296	C21H44	000629-94-7	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070819\
Data File : BF115428.D
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Operator : HP/JU
Sample : K3681-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PILEA-07-01-19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

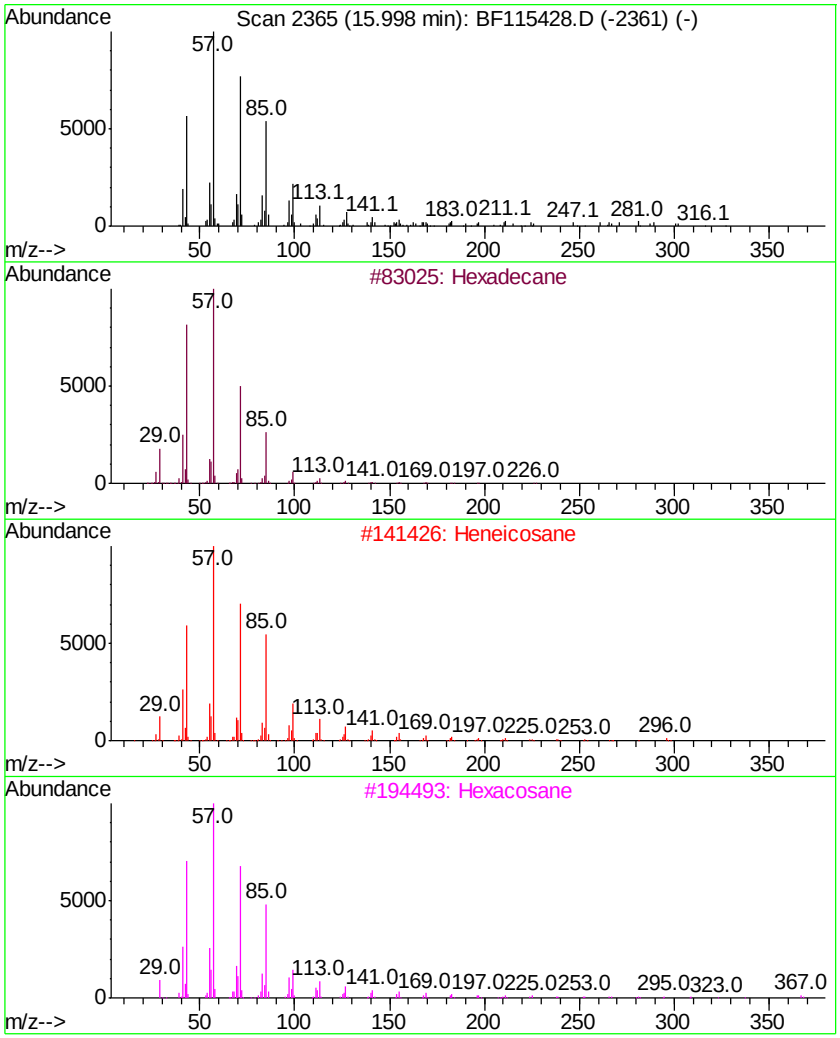
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

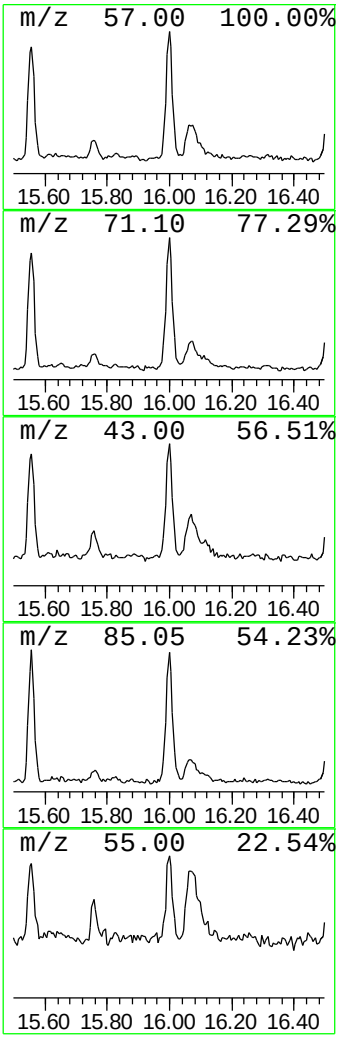
****

Peak Number 10 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.00	2.92 ng	176881	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	Hexacosane	366	C26H54	000630-01-3	90
4	Heptadecane	240	C17H36	000629-78-7	90
5	Tetratetracontane	619	C44H90	007098-22-8	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070819\
Data File : BF115428.D
Acq On : 9 Jul 2019 1:37
Operator : HP/JU
Sample : K3681-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PILEA-07-01-19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.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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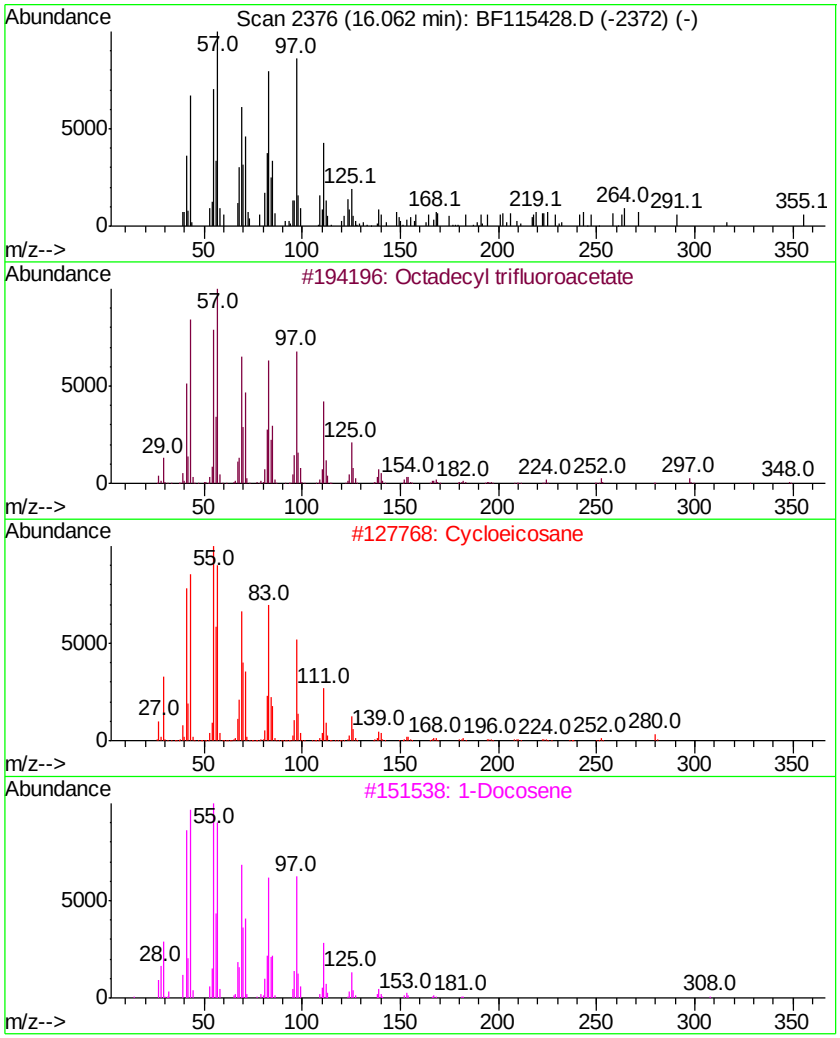
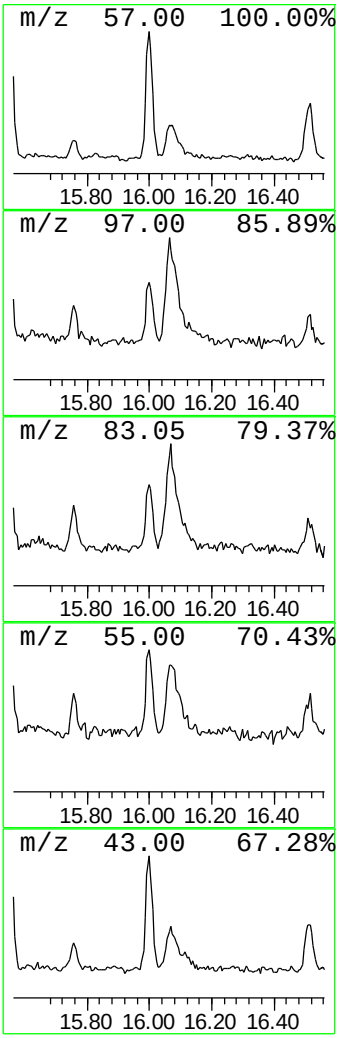
Peak Number 11 Octadecyl trifluoroacetate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.06	2.67 ng	162293	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90
2	Cycloeicosane	280	C20H40	000296-56-0	90
3	1-Docosene	308	C22H44	001599-67-3	87
4	Bacteriochlorophyll-c-stearyl	841	C52H72MgN4O4	1000164-49-7	87
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF070819\
Data File : BF115428.D
Acq On : 9 Jul 2019 1:37
Operator : HP/JU
Sample : K3681-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PILEA-07-01-19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.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...	2.20	31.1	ng	1758420	1	6.89	1132550	20.0
unknown6.66	6.66	70.3	ng	3981900	1	6.89	1132550	20.0
n-Hexadecanoic acid	11.93	3.1	ng	260826	4	11.41	1689920	20.0
Cinnamyl cinnamate	13.74	7.2	ng	462704	5	14.04	1288960	20.0
2- Chloropropioni...	13.90	9.2	ng	592091	5	14.04	1288960	20.0
Chloroacetic acid...	14.54	2.5	ng	162367	5	14.04	1288960	20.0
Heneicosane	14.83	2.1	ng	126588	6	15.51	1213550	20.0
Nonadecane	15.17	2.7	ng	163229	6	15.51	1213550	20.0
Hexadecane	16.00	2.9	ng	176881	6	15.51	1213550	20.0
Octadecyl trifluo...	16.06	2.7	ng	162293	6	15.51	1213550	20.0