LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112219\
Data File : BF117947.D
Acq On : 23 Nov 2019 4:34
Operator : JU
Sample : K5839-01 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NW-01

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-BF111319.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	2.175	10	15	21	rVB	235520	288738	21.49%	1.600%
2	3.993	319	324	332	rBV	17446	23076	1.72%	0.128%
3	5.104	509	513	520	rVB	237729	229959	17.11%	1.274%
4	5.510	578	582	585	rBV	1406360	1189339	88.51%	6.592%
5	6.522	749	754	761	rBV	1339642	1267927	94.36%	7.027%
6	6.616	767	770	773	rVB	39651	27865	2.07%	0.154%
7	6.669	775	779	782	rBV	1611400	1303857	97.03%	7.226%
8	6.904	815	819	823	rBV	1258225	1006387	74.90%	5.578%
9	7.057	842	845	849	rBV	1168755	1064220	79.20%	5.898%
10	7.463	910	914	917	rBV	888119	725094	53.96%	4.019%
11	7.498	919	920	924	rVB	20209	17210	1.28%	0.095%
12	7.539	924	927	932	rVB5	12921	19373	1.44%	0.107%
13	8.192	1032	1038	1041	rBV	1495000	1245598	92.70%	6.903%
14	8.251	1045	1048	1051	rVB2	37482	34712	2.58%	0.192%
15	8.486	1080	1088	1092	rBV6	24222	38872	2.89%	0.215%
16	8.569	1099	1102	1107	rVB5	12226	17314	1.29%	0.096%
17	8.610	1107	1109	1112	rBV	42801	39753	2.96%	0.220%
18	8.781	1136	1138	1143	rBV	62048	52699	3.92%	0.292%
19	9.104	1190	1193	1197	rVB5	10798	16935	1.26%	0.094%
20	9.216	1209	1212	1217	rVB	41820	33677	2.51%	0.187%
21	9.269	1217	1221	1224	rBV	1720797	1343711	100.00%	7.447%
22	9.351	1232	1235	1243	rVB	61842	61180	4.55%	0.339%
23	9.663	1285	1288	1292	rBV	183075	155848	11.60%	0.864%
24	9.880	1318	1325	1330	rVB3	28713	42039	3.13%	0.233%
25	9.951	1334	1337	1341	rBV	1255466	1162150	86.49%	6.441%
26	10.739	1468	1471	1480	rBV	751161	689413	51.31%	3.821%
27	10.851	1487	1490	1497	rVB3	30758	39981	2.98%	0.222%
28	11.445	1587	1591	1595	rBV	1265204	1036442	77.13%	5.744%
29	11.969	1676	1680	1691	rBV	293500	308748	22.98%	1.711%
30	12.663	1794	1798	1799	rBV2	94616	99727	7.42%	0.553%
31	12.674	1799	1800	1809	rVV	116941	158781	11.82%	0.880%
32	12.757	1811	1814	1824	rVB	112901	142593	10.61%	0.790%
33	12.892	1834	1837	1842	rVB	34434	44527	3.31%	0.247%
34	13.033	1857	1861	1864	rBV	1380260	1120009	83.35%	6.207%

LSC Area Percent Report

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Operator : JU
Sample : K5839-01 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NW-01

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-BF111319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.533	1944	1946	1949	rVB2	19410	17937	1.33%	0.099%
36	13.939	2011	2015	2021	rBV2	94375	156700	11.66%	0.868%
37	14.092	2037	2041	2045	rBV	1125371	1045246	77.79%	5.793%
38	14.257	2066	2069	2071	rBV	38896	36237	2.70%	0.201%
39	14.563	2117	2121	2128	rBV	64556	110203	8.20%	0.611%
40	14.874	2171	2174	2179	rBV	77092	85669	6.38%	0.475%
41	15.027	2198	2200	2203	rVB2	42710	40534	3.02%	0.225%
42	15.227	2231	2234	2238	rBV	98187	117543	8.75%	0.651%
43	15.598	2292	2297	2301	rBV	731272	986378	73.41%	5.467%
44	15.839	2336	2338	2341	rVB3	31647	26139	1.95%	0.145%
45	16.086	2377	2380	2385	rVB	63598	92990	6.92%	0.515%
46	16.368	2425	2428	2431	rBV5	32101	50013	3.72%	0.277%
47	16.480	2445	2447	2450	rBV3	23259	27437	2.04%	0.152%
48	16.609	2464	2469	2476	rBV3	50125	113111	8.42%	0.627%
49	16.756	2492	2494	2496	rBV3	26447	25270	1.88%	0.140%
50	16.962	2527	2529	2532	rBV4	20826	30318	2.26%	0.168%
51	17.245	2574	2577	2578	rBV2	26558	33929	2.53%	0.188%

Sum of corrected areas: 18043408

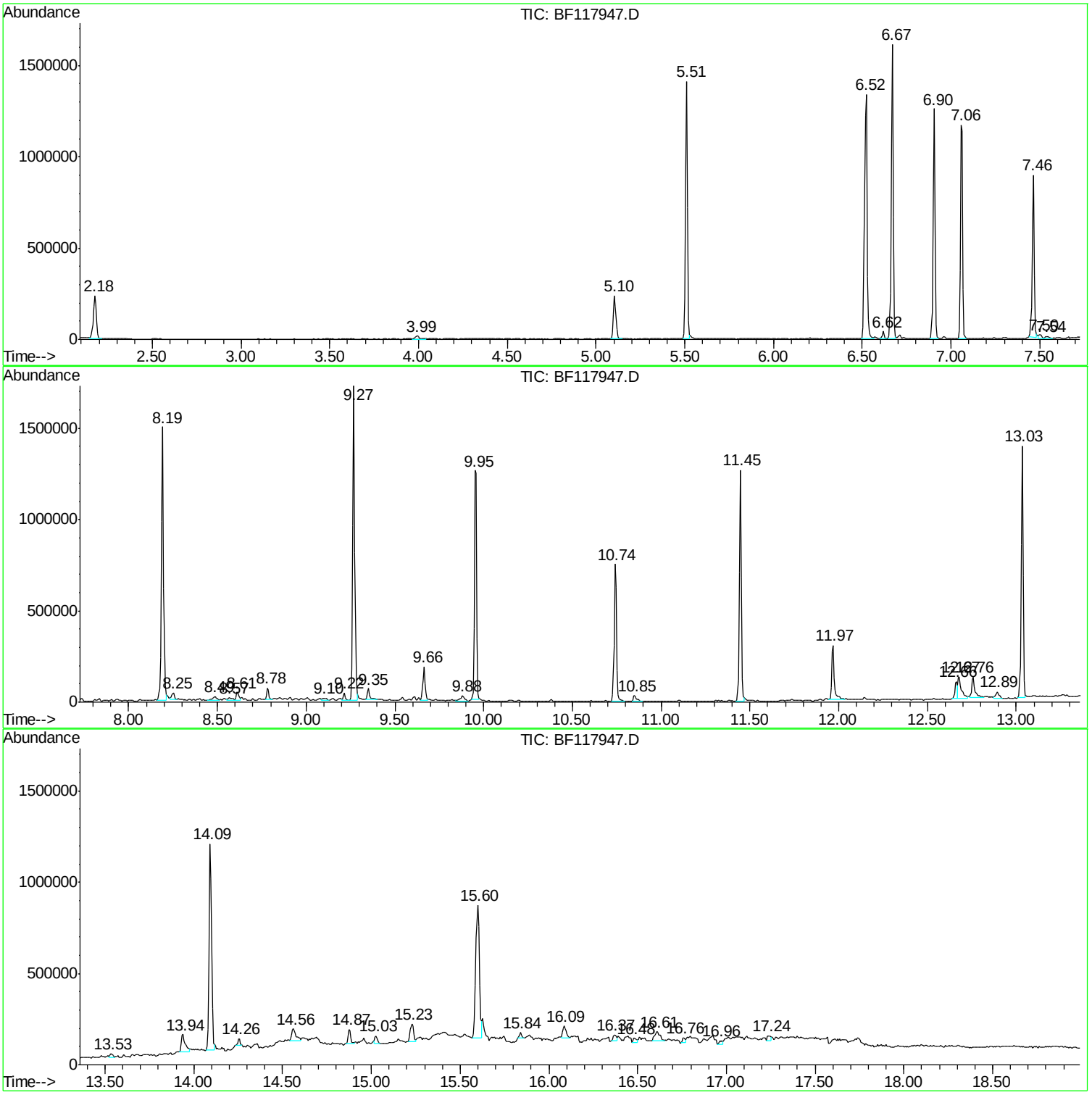
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112219\
Data File : BF117947.D
Acq On : 23 Nov 2019 4:34
Operator : JU
Sample : K5839-01 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PHIPPS-BH-NW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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\BF112219\
Data File : BF117947.D
Acq On : 23 Nov 2019 4:34
Operator : JU
Sample : K5839-01 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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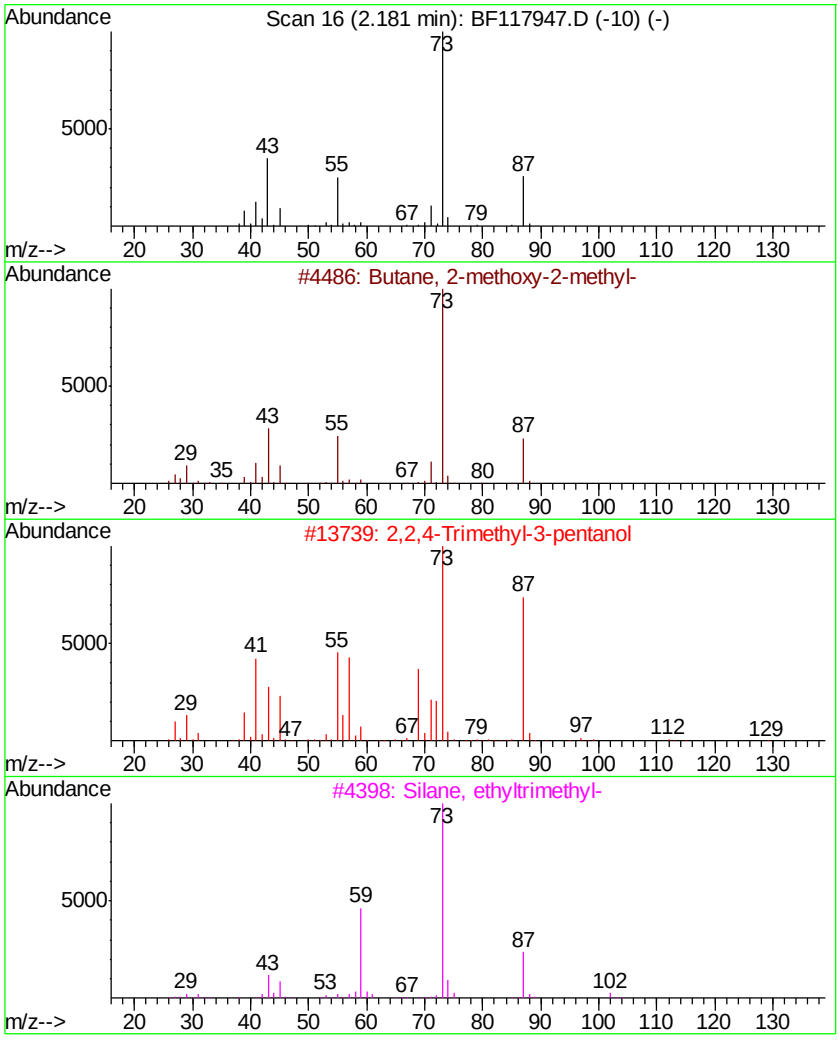
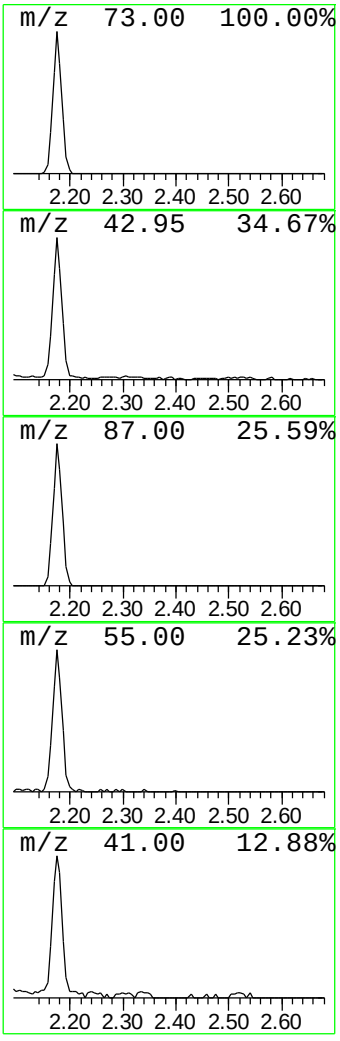
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	5.74 ng	288738	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
4	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





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Data File : BF117947.D
Acq On : 23 Nov 2019 4:34
Operator : JU
Sample : K5839-01 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

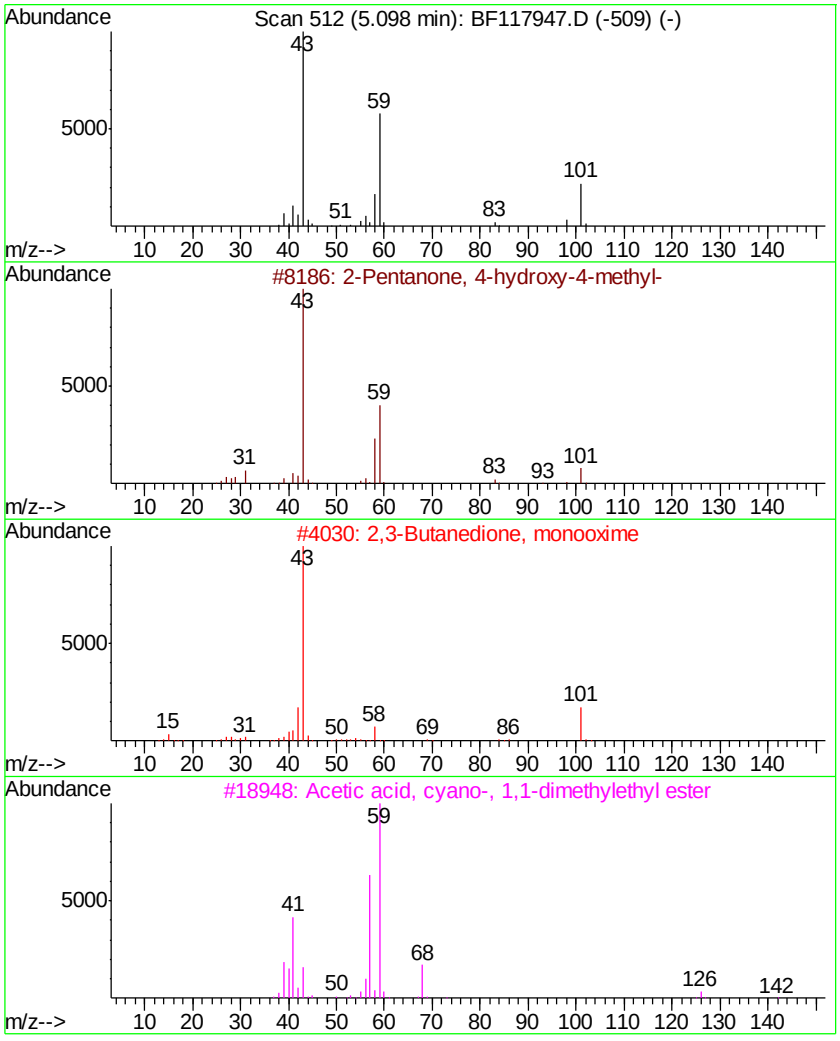
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

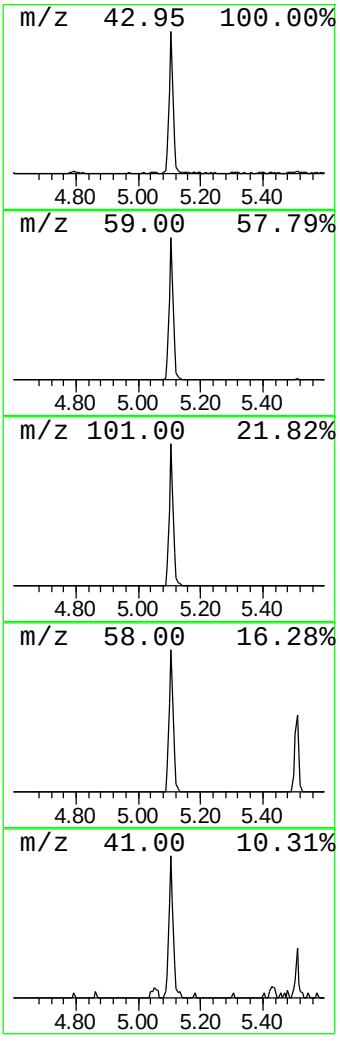
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	4.57 ng	229959	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Butane	58	C4H10	000106-97-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112219\
Data File : BF117947.D
Acq On : 23 Nov 2019 4:34
Operator : JU
Sample : K5839-01 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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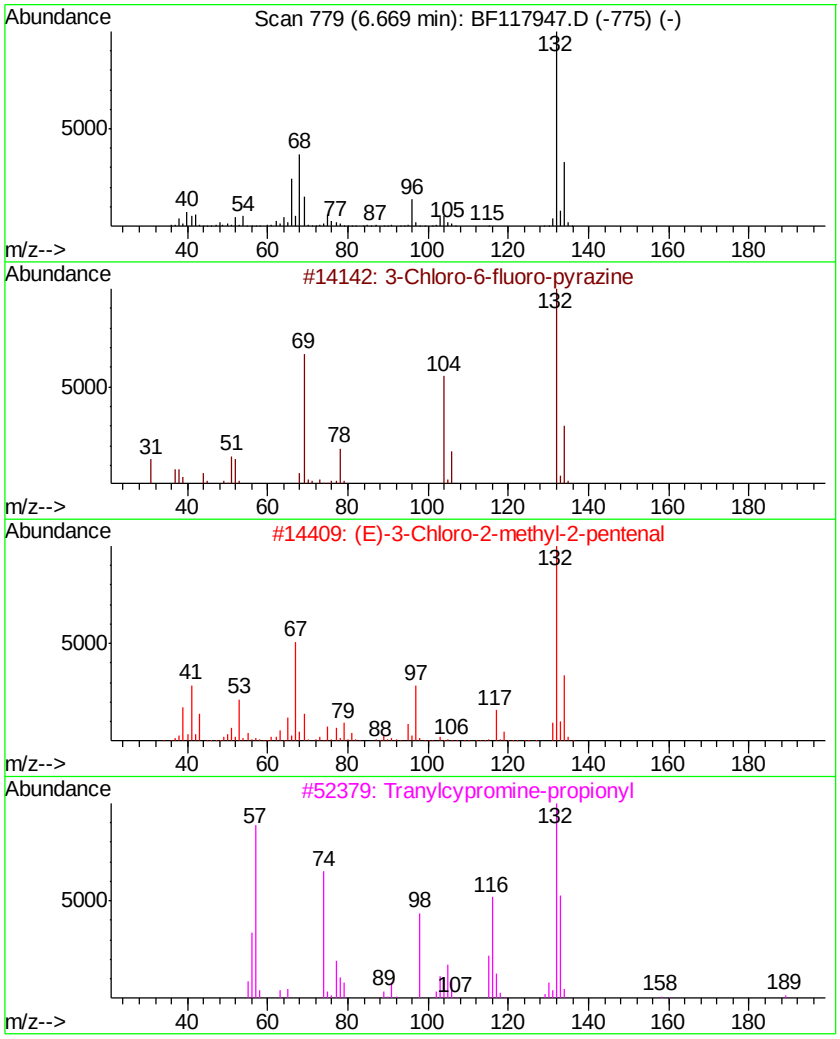
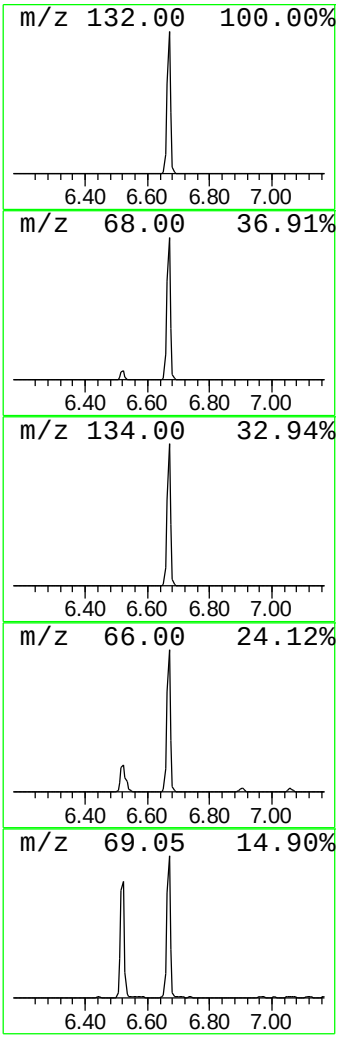
Peak Number 3 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	25.91 ng	1303860	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

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Sample : K5839-01 2X
Misc :
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Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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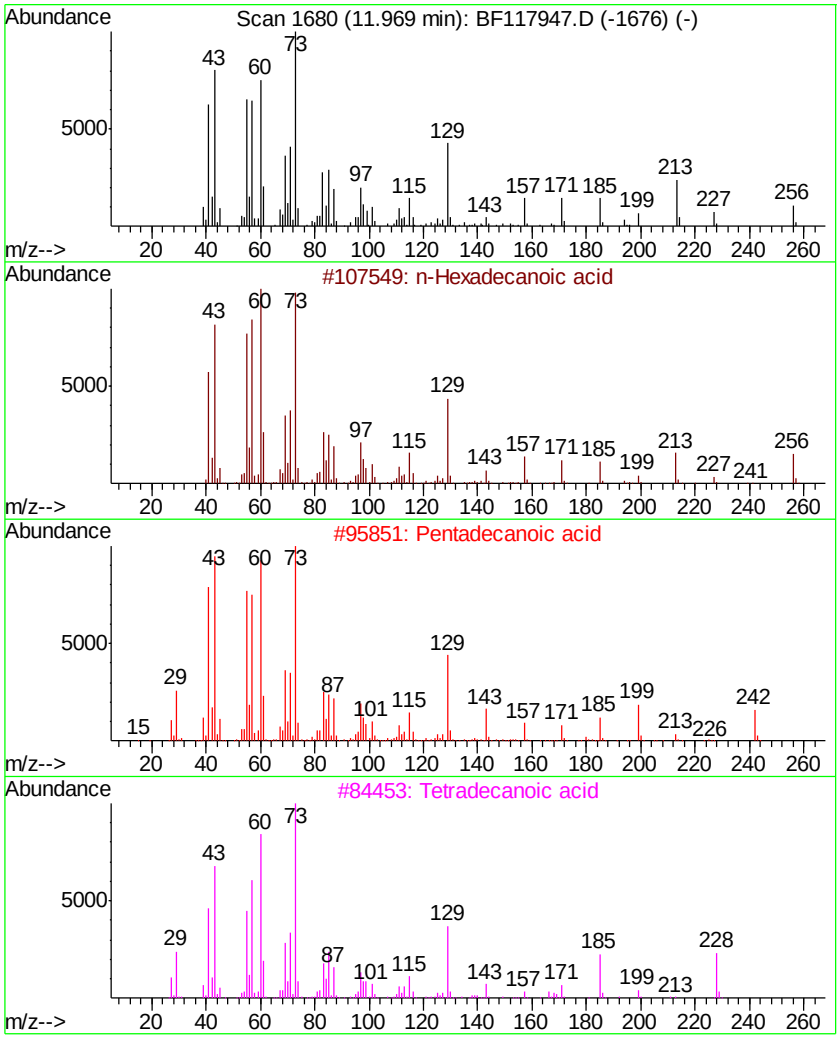
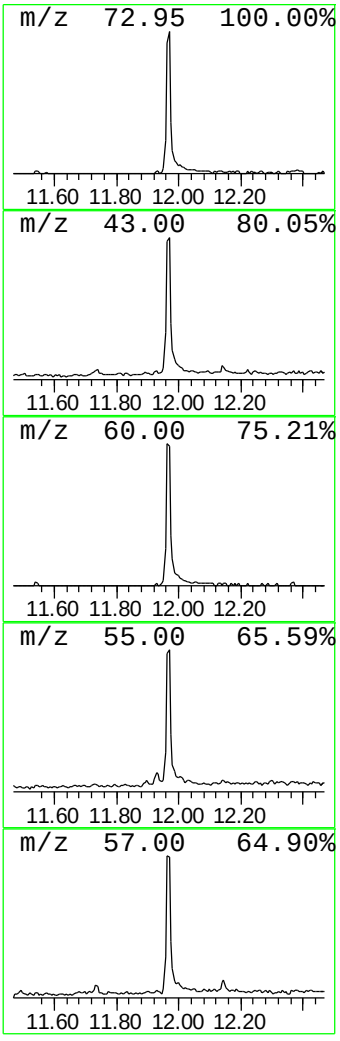
Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.97	5.96 ng	308748	Phenanthrene-d10	11.45

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	89
5	Ether, dodecyl isopropyl	228	C15H32O	029379-42-8	20





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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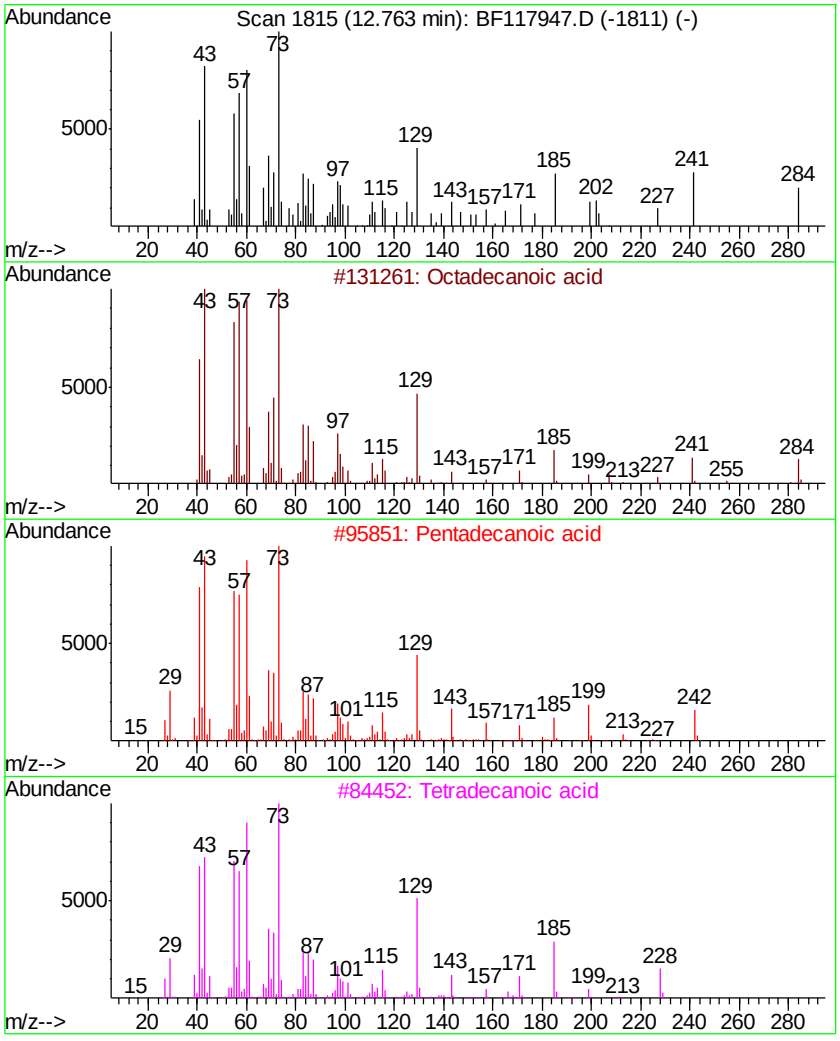
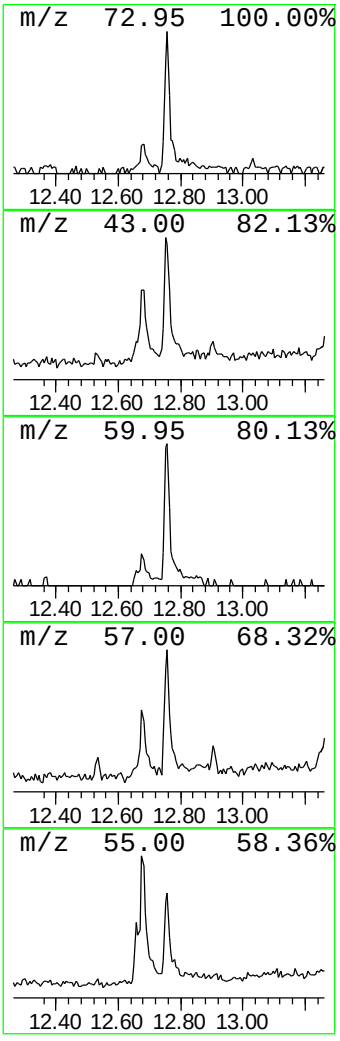
Peak Number 7 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.76	2.75 ng	142593	Phenanthrene-d10	11.45

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	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5	Tridecanoic acid	214	C13H26O2	000638-53-9	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112219\
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Acq On : 23 Nov 2019 4:34
Operator : JU
Sample : K5839-01 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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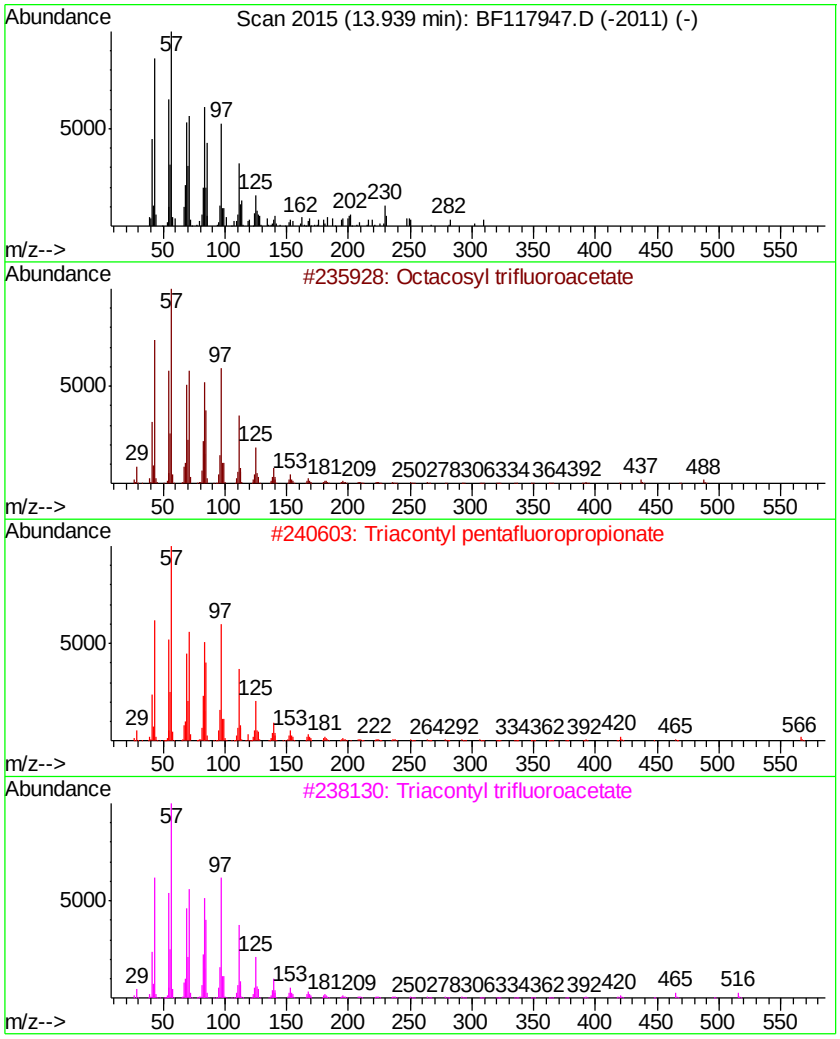
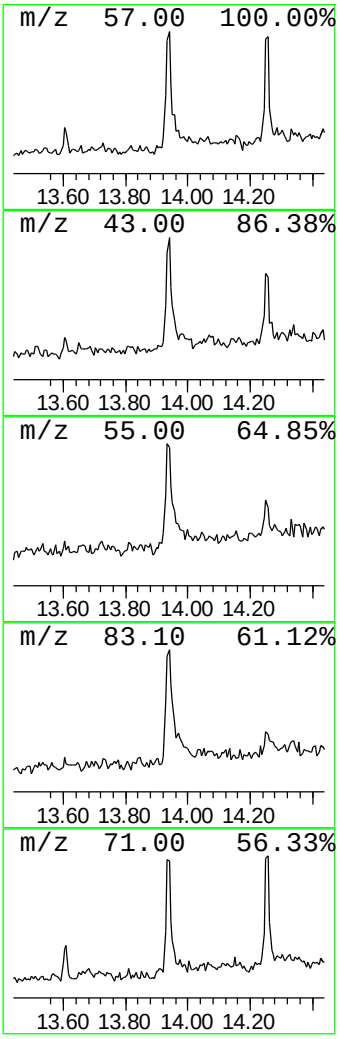
Peak Number 8 Octacosyl trifluoroacetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	3.00 ng	156700	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	87
2	Triacontyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	83
3	Triacontyl trifluoroacetate	534	C32H61F3O2	1000351-75-7	83
4	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	83
5	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	80





Library Search Compound Report

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Data File : BF117947.D
Acq On : 23 Nov 2019 4:34
Operator : JU
Sample : K5839-01 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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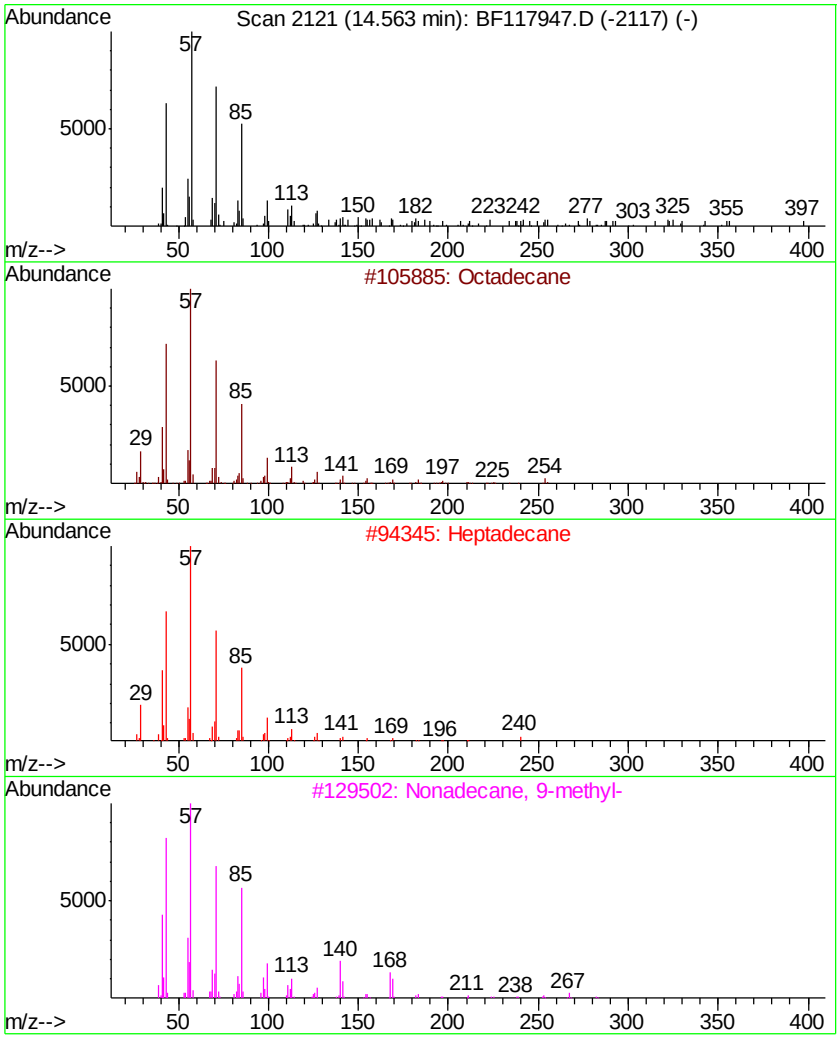
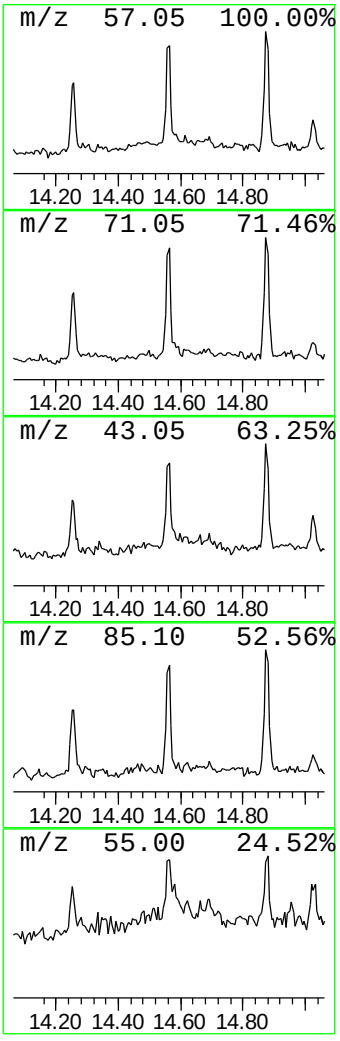
Peak Number 9 Octadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	2.11 ng	110203	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	96
2	Heptadecane	240	C17H36	000629-78-7	93
3	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	93
4	Pentadecane	212	C15H32	000629-62-9	92
5	Tetracosane	338	C24H50	000646-31-1	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112219\
Data File : BF117947.D
Acq On : 23 Nov 2019 4:34
Operator : JU
Sample : K5839-01 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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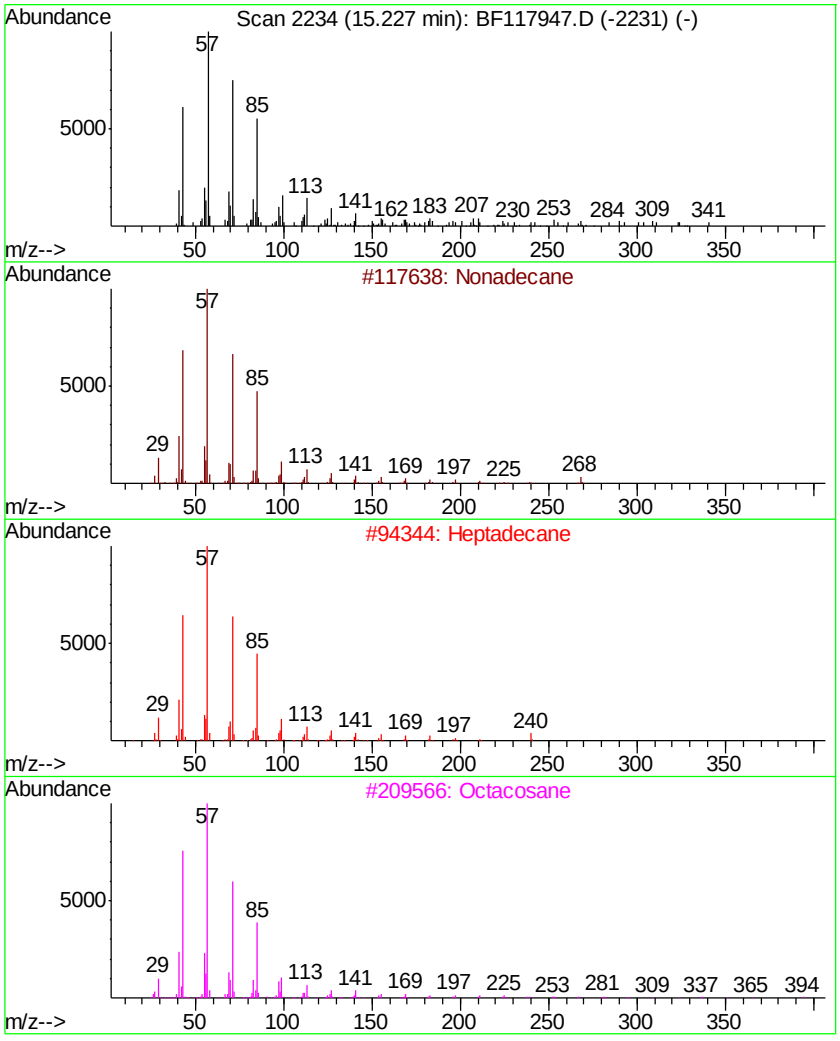
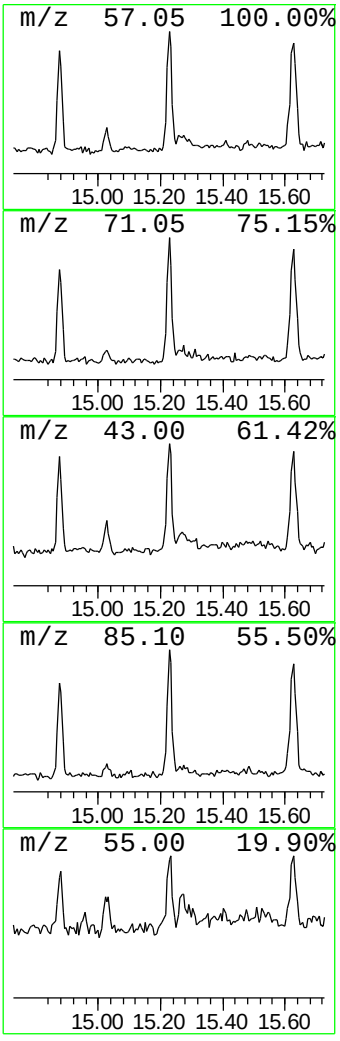
Peak Number 10 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.23	2.38 ng	117543	Perylene-d12	15.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	97
2	Heptadecane	240	C17H36	000629-78-7	95
3	Octacosane	394	C28H58	000630-02-4	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Triacontane	422	C30H62	000638-68-6	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112219\
Data File : BF117947.D
Acq On : 23 Nov 2019 4:34
Operator : JU
Sample : K5839-01 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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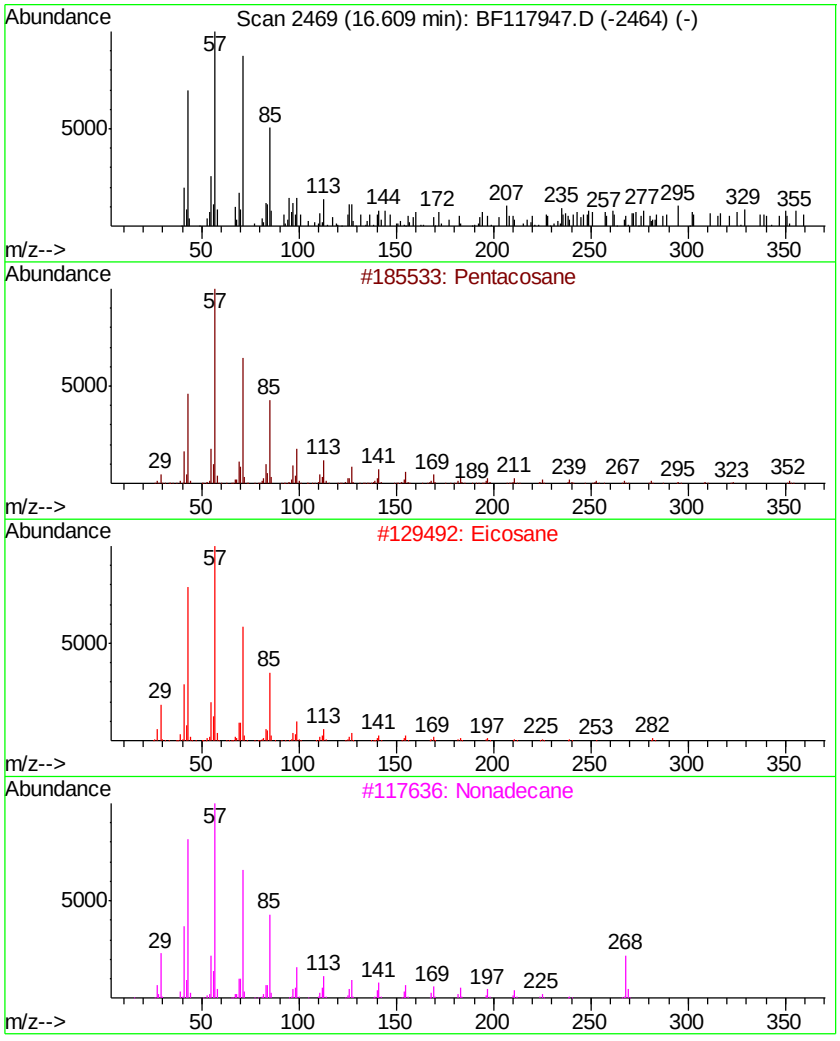
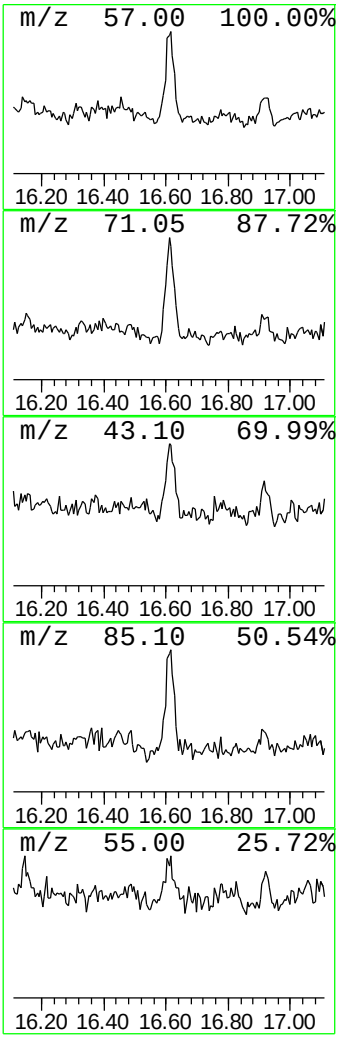
Peak Number 11 Pentacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.61	2.29 ng	113111	Perylene-d12	15.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	86
2	Eicosane	282	C20H42	000112-95-8	70
3	Nonadecane	268	C19H40	000629-92-5	62
4	Hexacosane	366	C26H54	000630-01-3	58
5	Undecane, 2-methyl-	170	C12H26	007045-71-8	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112219\
Data File : BF117947.D
Acq On : 23 Nov 2019 4:34
Operator : JU
Sample : K5839-01 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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...	2.18	5.7	ng	288738	1	6.90	1006390	20.0
2-Pentanone, 4-hy...	5.10	4.6	ng	229959	1	6.90	1006390	20.0
unknown6.67	6.67	25.9	ng	1303860	1	6.90	1006390	20.0
n-Hexadecanoic acid	11.97	6.0	ng	308748	4	11.45	1036440	20.0
Octadecanoic acid	12.76	2.8	ng	142593	4	11.45	1036440	20.0
Octacosyl trifluo...	13.94	3.0	ng	156700	5	14.09	1045250	20.0
Octadecane	14.56	2.1	ng	110203	5	14.09	1045250	20.0
Nonadecane	15.23	2.4	ng	117543	6	15.60	986378	20.0
Pentacosane	16.61	2.3	ng	113111	6	15.60	986378	20.0