LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
Data File : BF117860.D
Acq On : 19 Nov 2019 15:36
Operator : JU
Sample : K5865-17
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-(4-6)

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	2.193	12	18	24	rVB	765479	971024	18.02%	1.976%
2	5.128	508	517	525	rBV	644124	752182	13.96%	1.530%
3	5.528	580	585	588	rBV	4195640	3823655	70.96%	7.779%
4	6.534	751	756	769	rBV	4072237	4281605	79.46%	8.711%
5	6.681	777	781	784	rBV	4700378	4256160	78.99%	8.659%
6	6.916	817	821	824	rBV	1550403	1248766	23.18%	2.541%
7	7.075	844	848	851	rVB	3724206	3373487	62.61%	6.863%
8	7.475	911	916	919	rBV	2966434	2624500	48.71%	5.339%
9	8.204	1036	1040	1043	rBV	1765852	1643260	30.50%	3.343%
10	9.281	1218	1223	1226	rBV	5964758	5153704	95.65%	10.485%
11	9.675	1286	1290	1293	rVB	660662	512962	9.52%	1.044%
12	9.963	1335	1339	1343	rBV	2192868	1978079	36.71%	4.024%
13	10.757	1469	1474	1477	rBV	3392079	3070809	56.99%	6.247%
14	11.457	1589	1593	1596	rBV	2545841	2138708	39.69%	4.351%
15	11.480	1596	1597	1600	rVV	268152	143747	2.67%	0.292%
16	11.522	1600	1604	1609	rVB3	88805	108222	2.01%	0.220%
17	11.957	1674	1678	1680	rBV	64566	79734	1.48%	0.162%
18	11.986	1680	1683	1686	rVB2	93417	115136	2.14%	0.234%
19	12.069	1694	1697	1700	rBV2	77027	86918	1.61%	0.177%
20	12.675	1796	1800	1805	rBV	497837	432632	8.03%	0.880%
21	12.769	1813	1816	1819	rBV	79751	88537	1.64%	0.180%
22	12.904	1834	1839	1841	rBV	470296	450293	8.36%	0.916%
23	13.051	1859	1864	1867	rBV	5908698	5388245	100.00%	10.962%
24	13.122	1871	1876	1880	rBV2	41858	76821	1.43%	0.156%
25	13.233	1892	1895	1898	rVB2	58359	62588	1.16%	0.127%
26	13.621	1956	1961	1965	rBV2	53953	77859	1.44%	0.158%
27	13.739	1978	1981	1986	rVB	55269	59739	1.11%	0.122%
28	13.951	2013	2017	2027	rBV5	186093	418500	7.77%	0.851%
29	14.104	2035	2043	2046	rBV	1906531	1927723	35.78%	3.922%
30	14.127	2046	2047	2053	rVB	224964	174191	3.23%	0.354%
31	14.269	2067	2071	2074	rBV	104443	99303	1.84%	0.202%
32	14.574	2119	2123	2127	rBV2	189083	206364	3.83%	0.420%
33	14.892	2173	2177	2181	rVB	201640	218387	4.05%	0.444%
34	14.968	2187	2190	2194	rBV	121442	130070	2.41%	0.265%

LSC Area Percent Report

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Acq On : 19 Nov 2019 15:36
Operator : JU
Sample : K5865-17
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-(4-6)

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	15.163	2218	2223	2226	rBV	156688	239335	4.44%	0.487%
36	15.245	2233	2237	2240	rBV	198480	229429	4.26%	0.467%
37	15.480	2273	2277	2283	rVV	89624	116038	2.15%	0.236%
38	15.539	2283	2287	2293	rVB	114507	148107	2.75%	0.301%
39	15.610	2294	2299	2303	rBV2	1155006	1445398	26.83%	2.941%
40	15.645	2303	2305	2313	rVB2	214717	257304	4.78%	0.523%
41	16.104	2378	2383	2390	rVB	148842	215552	4.00%	0.439%
42	16.639	2470	2474	2479	rVB2	84259	145281	2.70%	0.296%
43	17.127	2554	2557	2567	rVB2	56577	111705	2.07%	0.227%
44	17.262	2578	2580	2586	rVB3	46686	70955	1.32%	0.144%

Sum of corrected areas: 49153014

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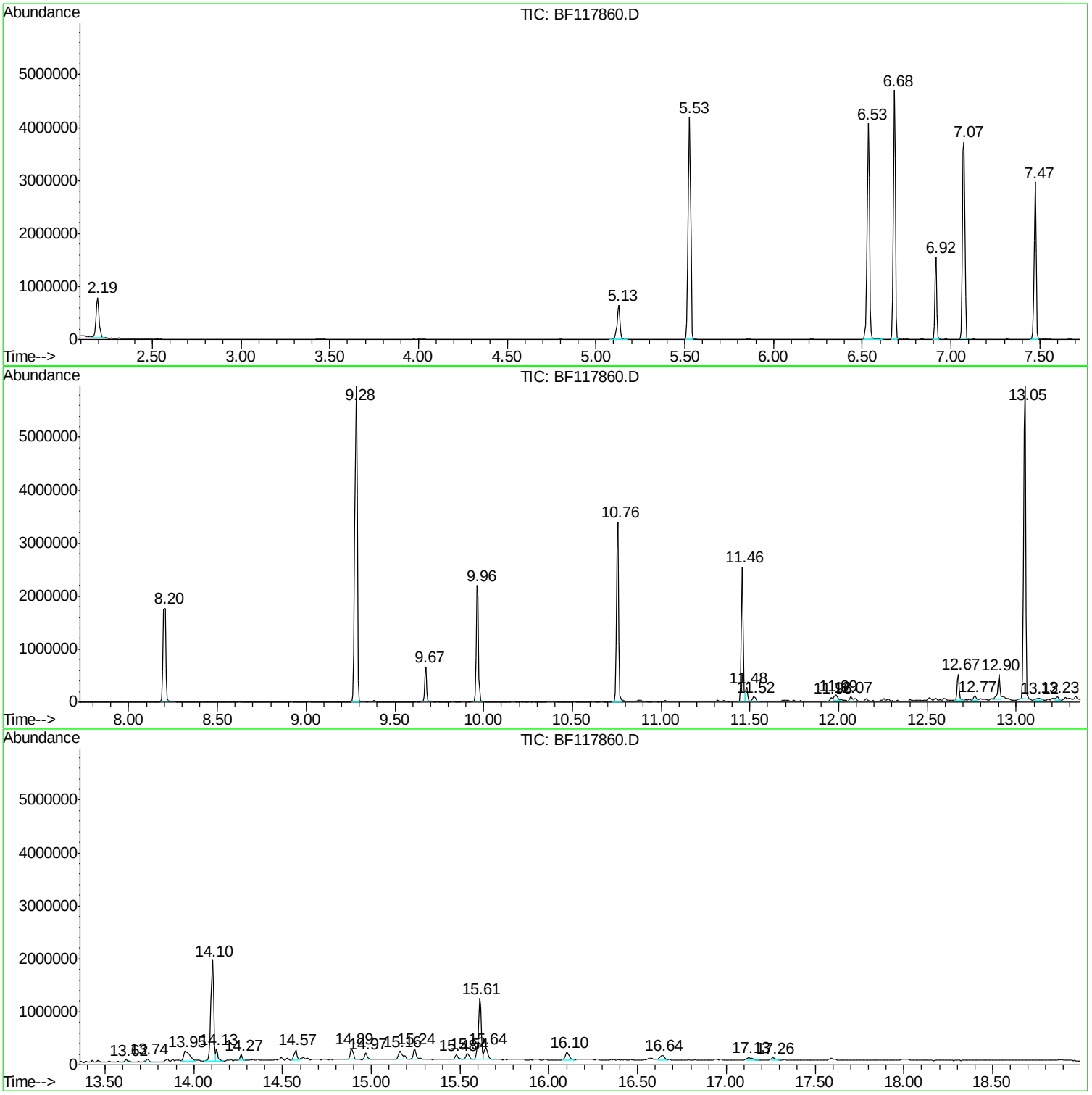
Instrument :
BNA_F
ClientSampleId :
2-(4-6)

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

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Data File : BF117860.D
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Sample : K5865-17
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ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-(4-6)

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

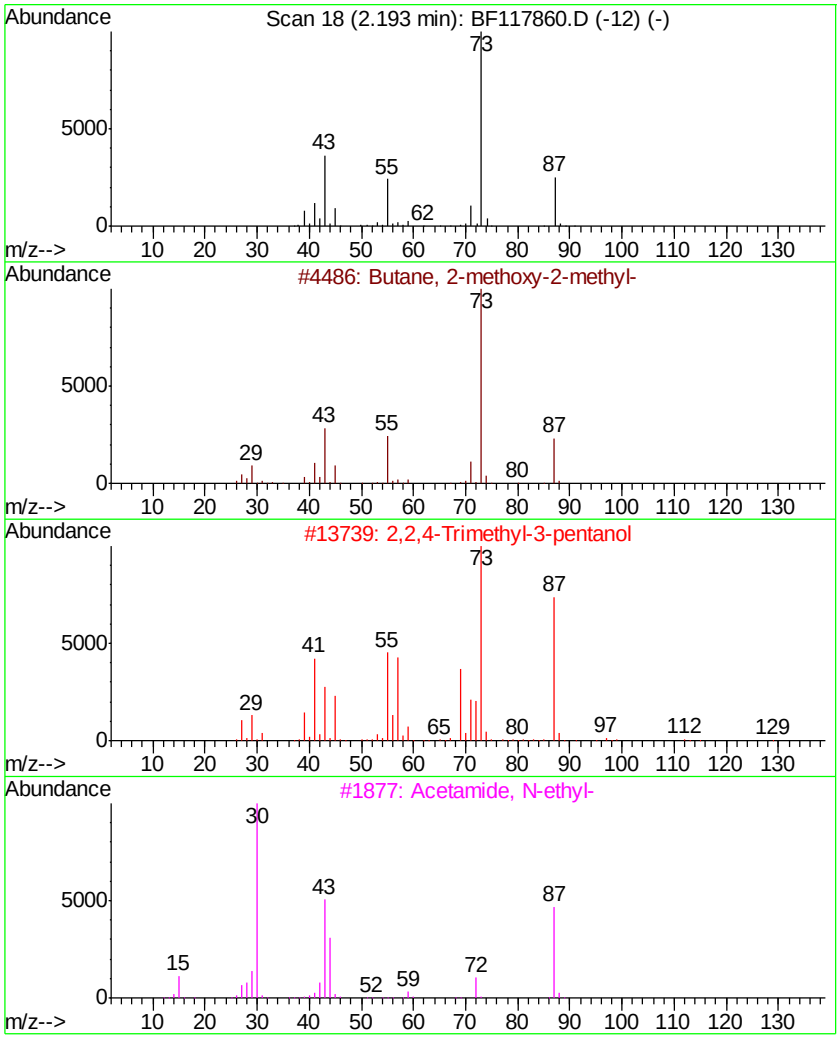
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

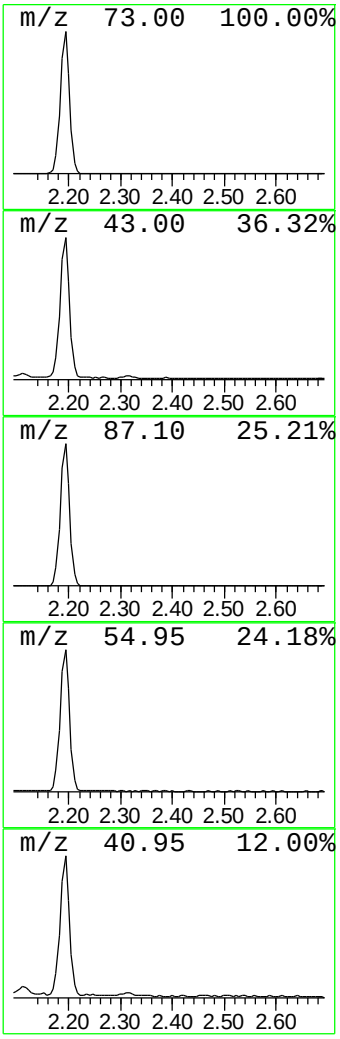
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.19	15.55 ng	971024	1,4-Dichlorobenzene-d4	6.92

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	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





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Operator : JU
Sample : K5865-17
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-(4-6)

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

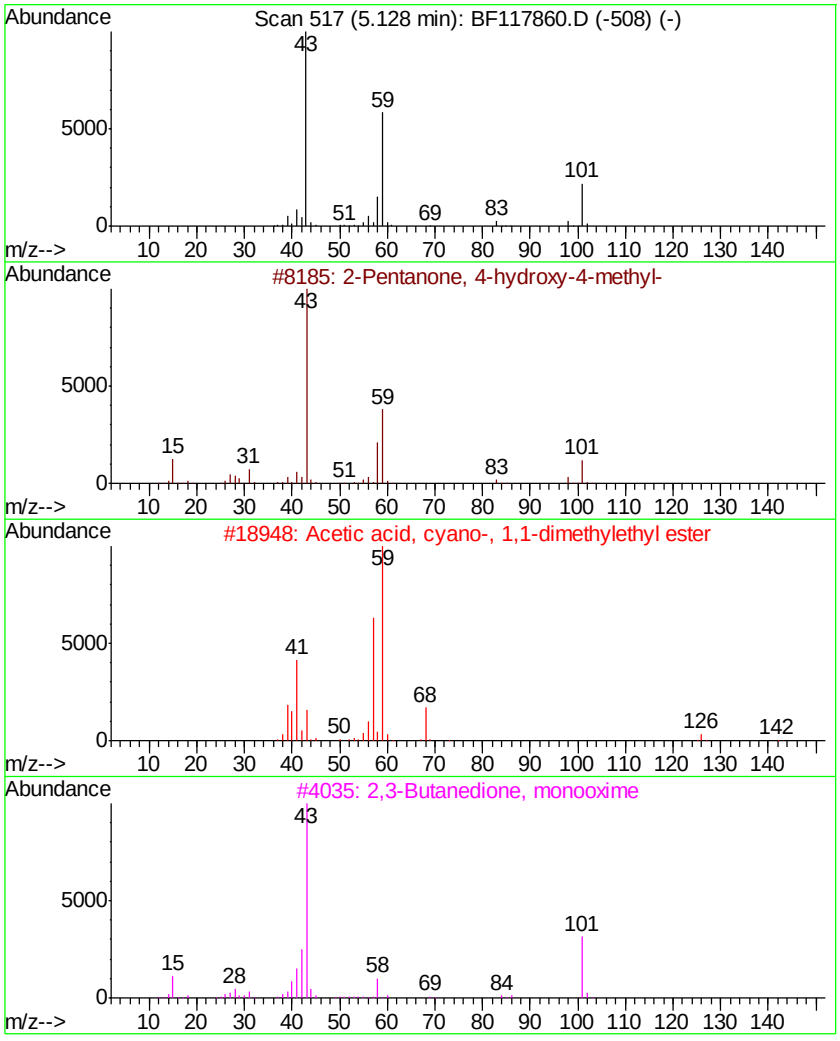
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

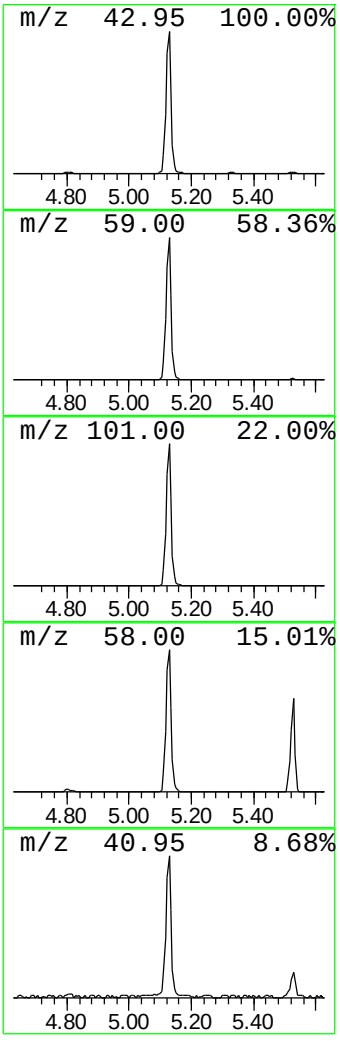
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	12.05 ng	752182	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
Data File : BF117860.D
Acq On : 19 Nov 2019 15:36
Operator : JU
Sample : K5865-17
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-(4-6)

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

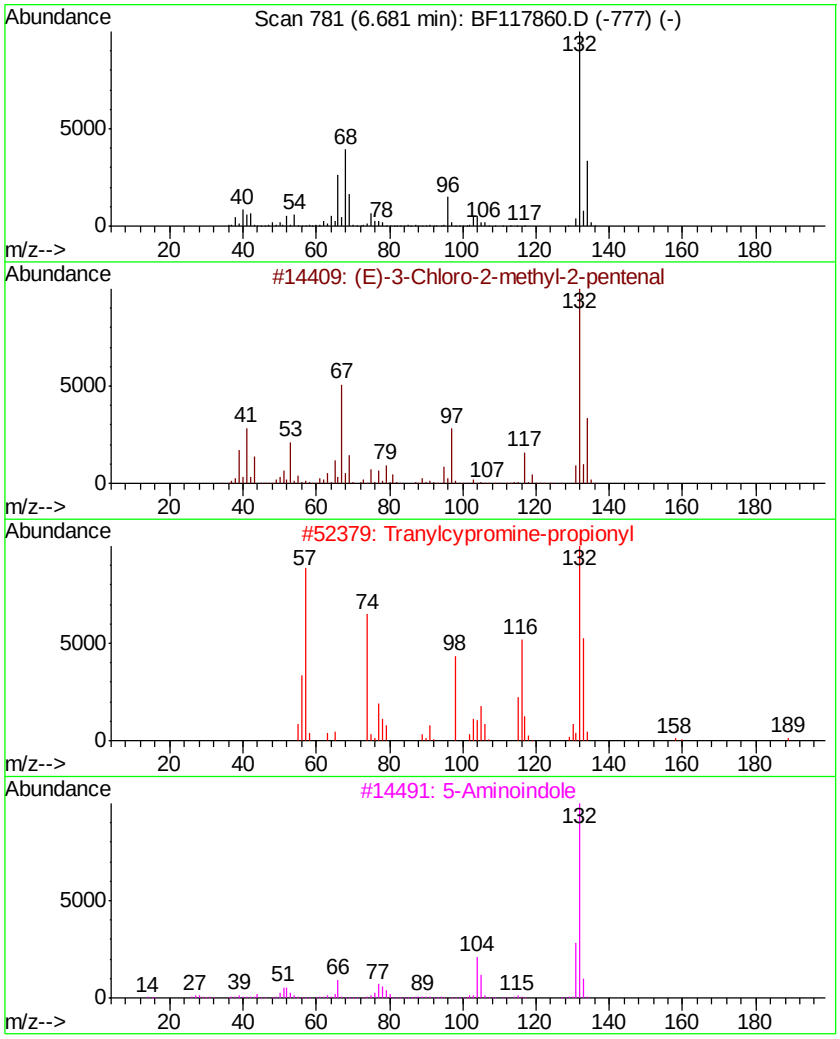
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

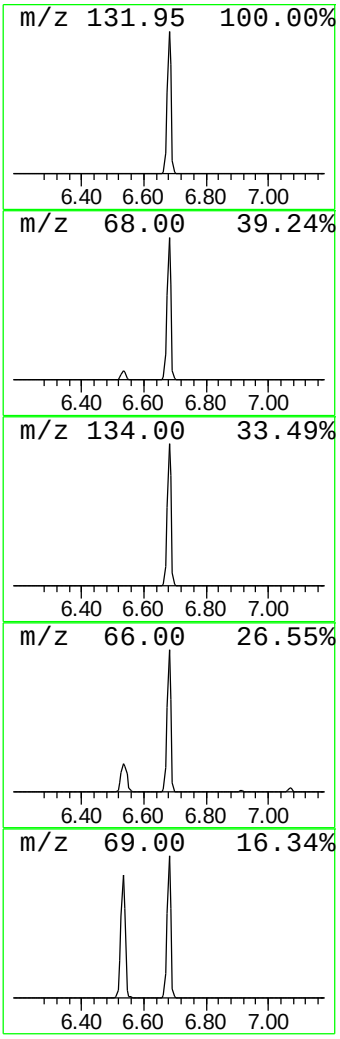
****

Peak Number 3 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	68.17 ng	4256160	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
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Sample : K5865-17
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-(4-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
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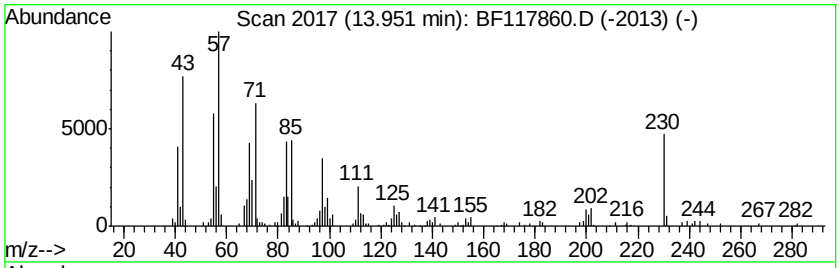
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

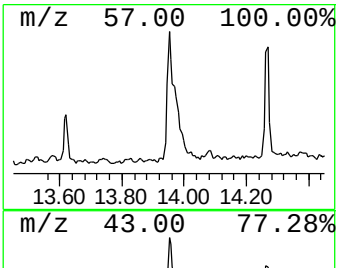
****

Peak Number 6 Oxalic acid, isobutyl hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	4.34 ng	418500	Chrysene-d12	14.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	81
2	Eicosane	282	C20H42	000112-95-8	80
3	Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	74
4	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	74
5	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	74





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Sample : K5865-17
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-(4-6)

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
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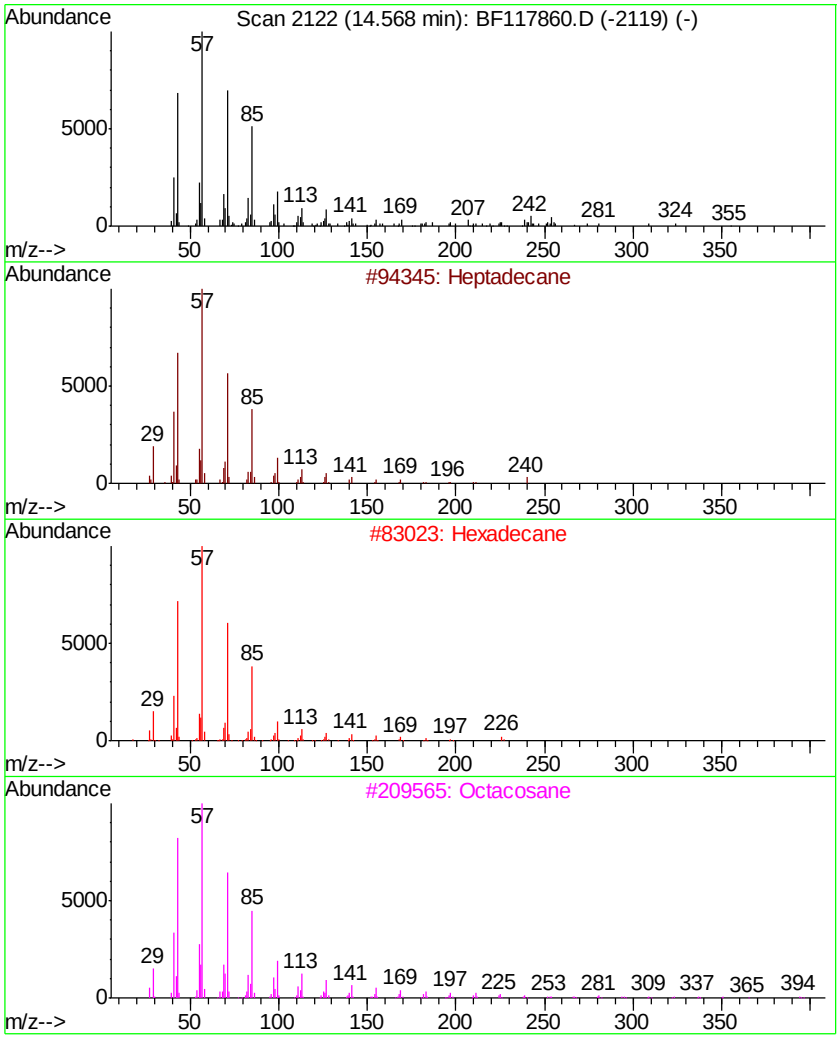
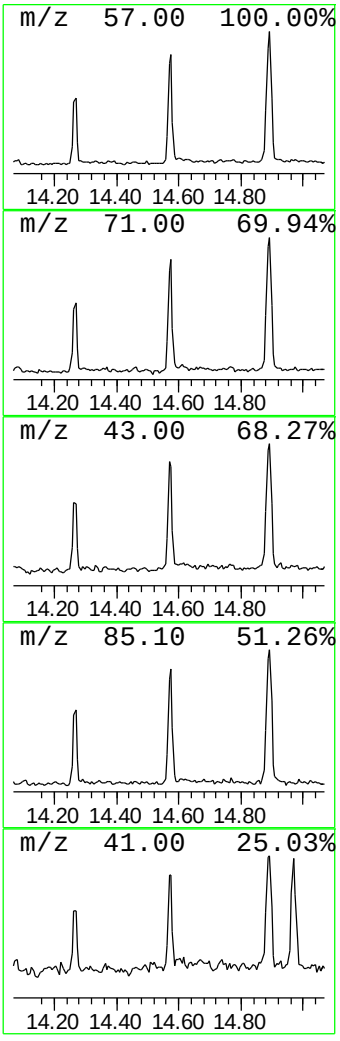
Peak Number 7 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	2.14 ng	206364	Chrysene-d12	14.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	95
2	Hexadecane	226	C16H34	000544-76-3	93
3	Octacosane	394	C28H58	000630-02-4	93
4	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	93
5	Octadecane	254	C18H38	000593-45-3	91





Library Search Compound Report

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ClientSampleId : 2-(4-6)

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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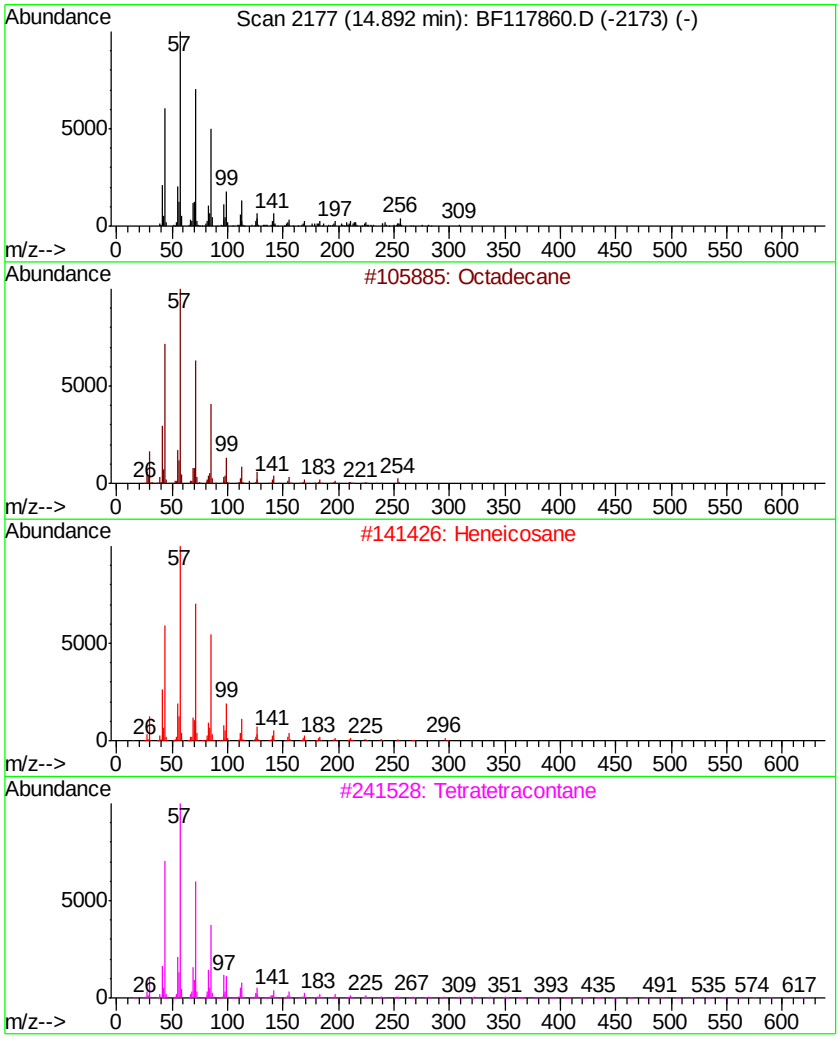
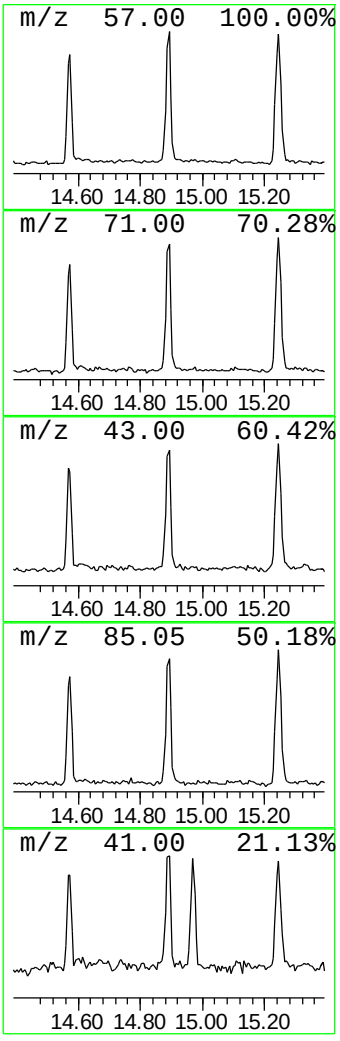
Peak Number 8 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	3.02 ng	218387	Perylene-d12	15.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	95
2	Heneicosane	296	C21H44	000629-94-7	90
3	Tetratetracontane	619	C44H90	007098-22-8	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Octacosane	394	C28H58	000630-02-4	87





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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-(4-6)

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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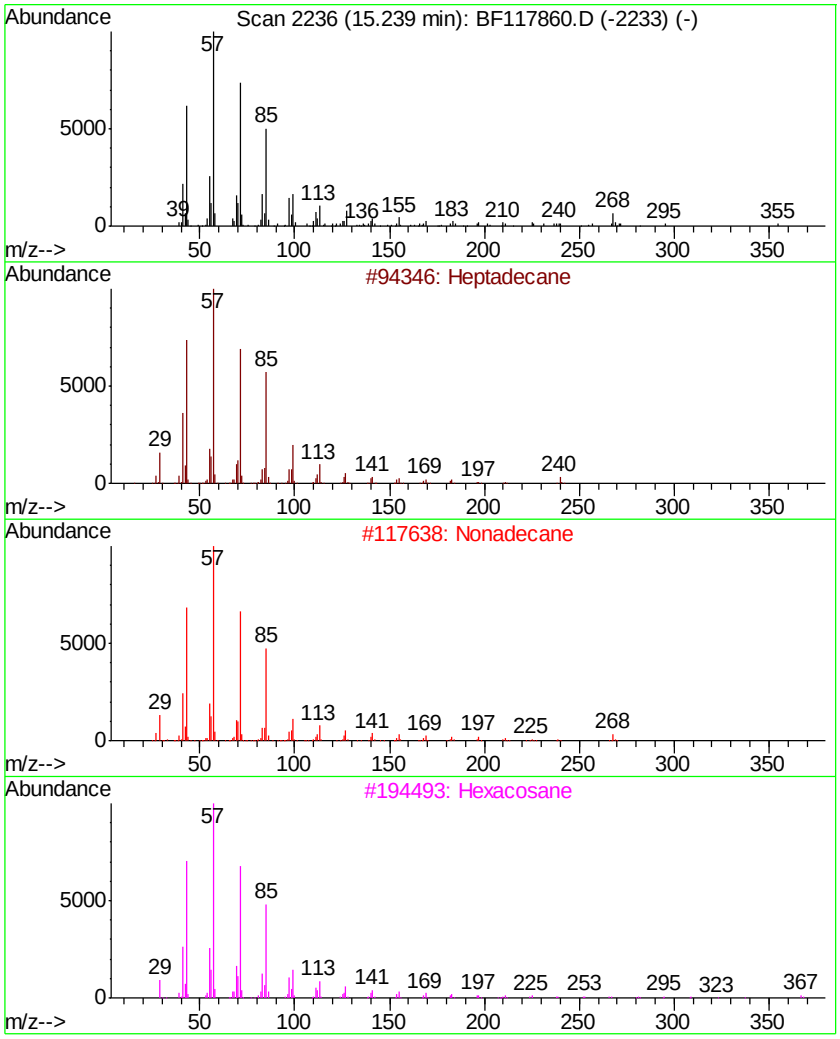
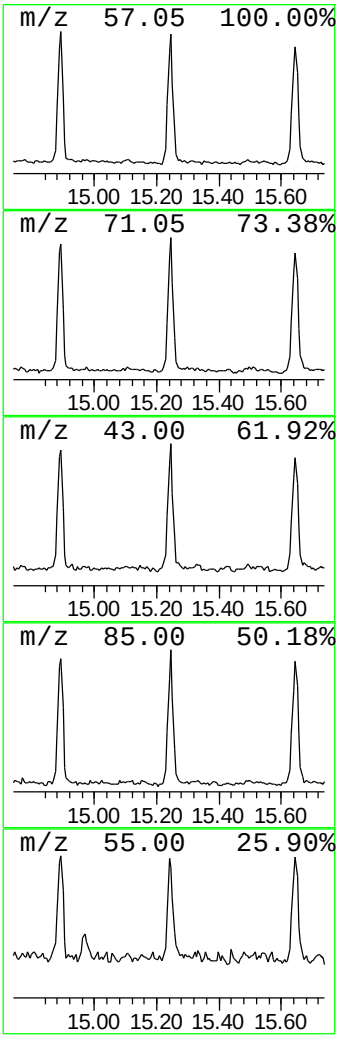
Peak Number 9 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.24	3.17 ng	229429	Perylene-d12	15.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	93
2	Nonadecane	268	C19H40	000629-92-5	93
3	Hexacosane	366	C26H54	000630-01-3	90
4	Octacosane	394	C28H58	000630-02-4	90
5	2-methyloctacosane	408	C29H60	1000376-72-8	90





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Data File : BF117860.D
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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-(4-6)

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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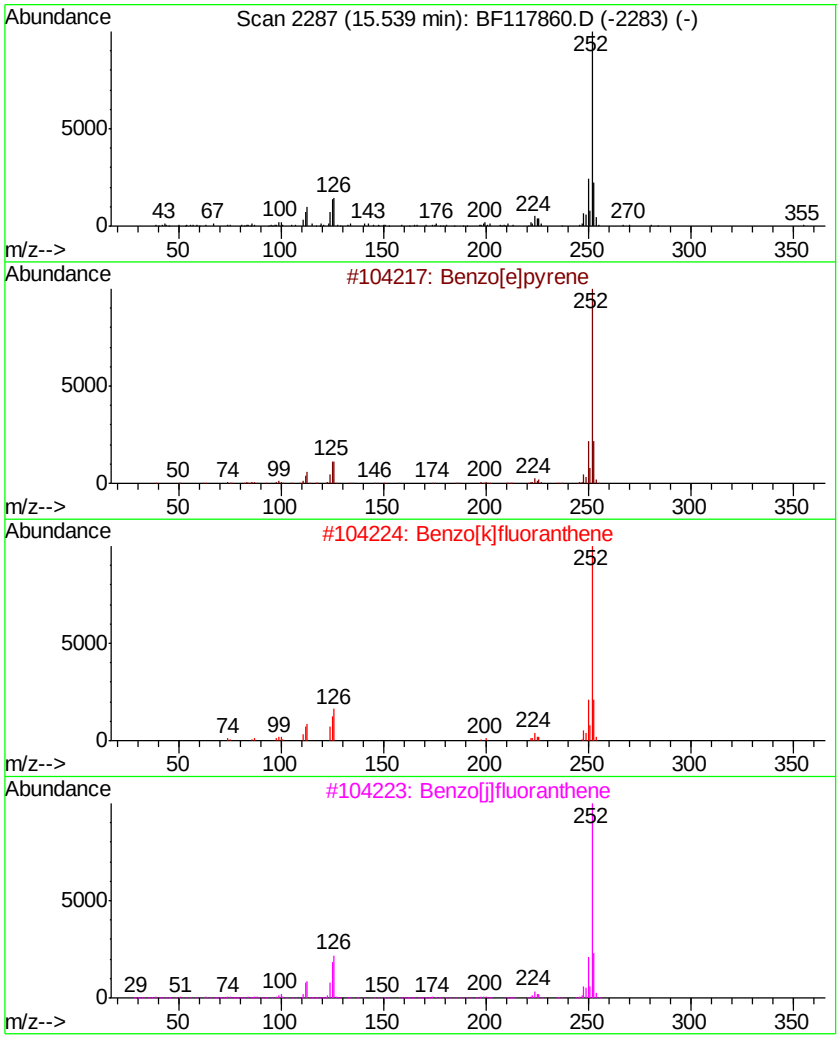
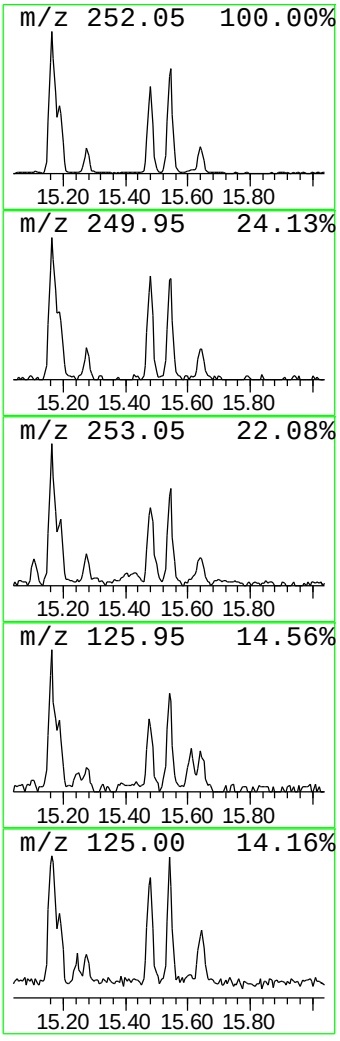
Peak Number 10 Benzo[e]pyrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.54	2.05 ng	148107	Perylene-d12	15.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	97
4	Perylene	252	C20H12	000198-55-0	96
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95





Library Search Compound Report

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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-(4-6)

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TIC Integration Parameters: LSCINT.P

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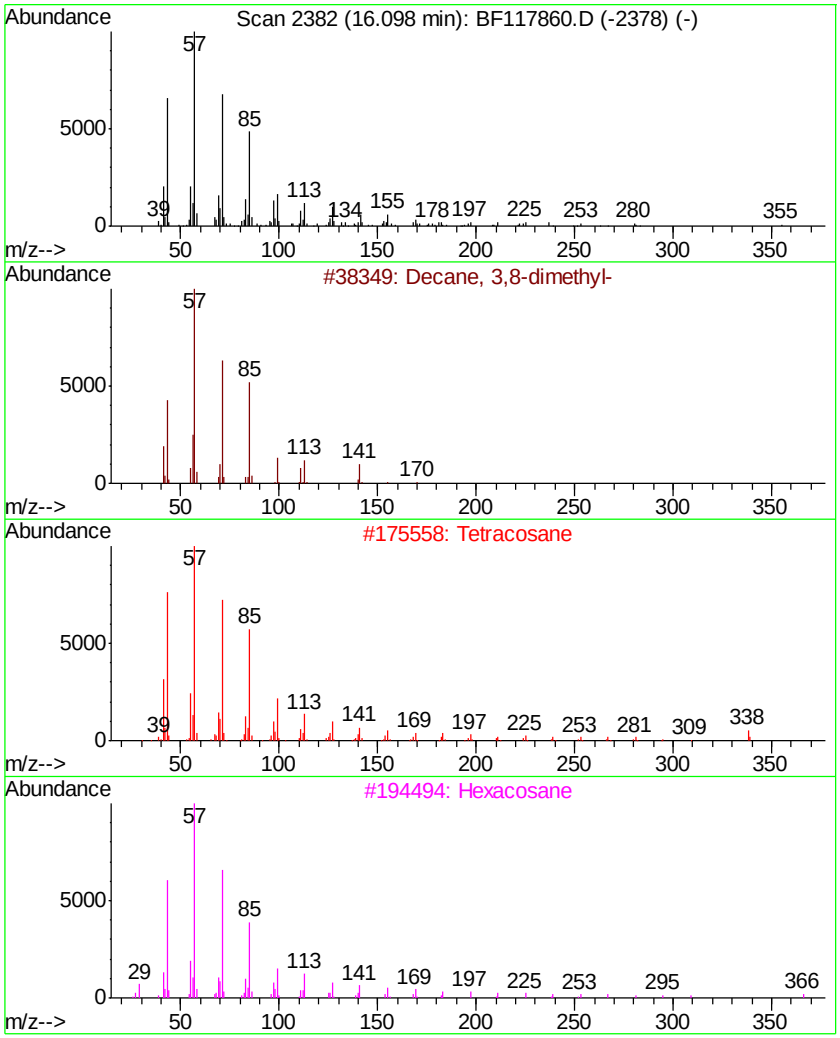
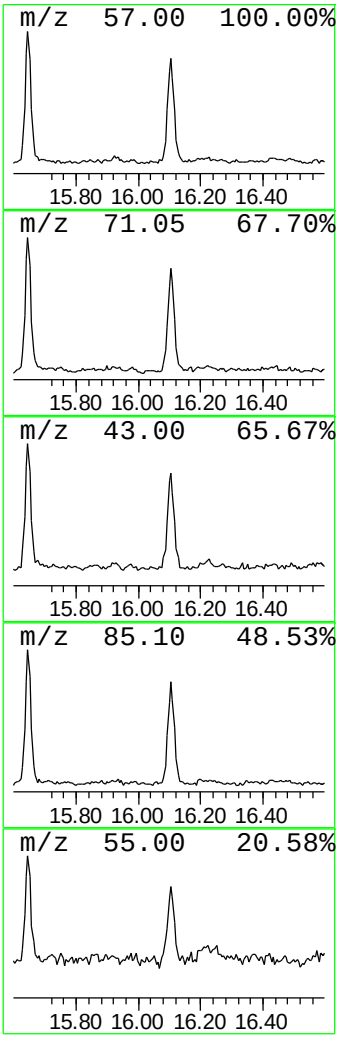
Peak Number 11 Decane, 3,8-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	2.98 ng	215552	Perylene-d12	15.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Tetratetracontane	619	C44H90	007098-22-8	90
5	Triacontane	422	C30H62	000638-68-6	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
Data File : BF117860.D
Acq On : 19 Nov 2019 15:36
Operator : JU
Sample : K5865-17
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-(4-6)

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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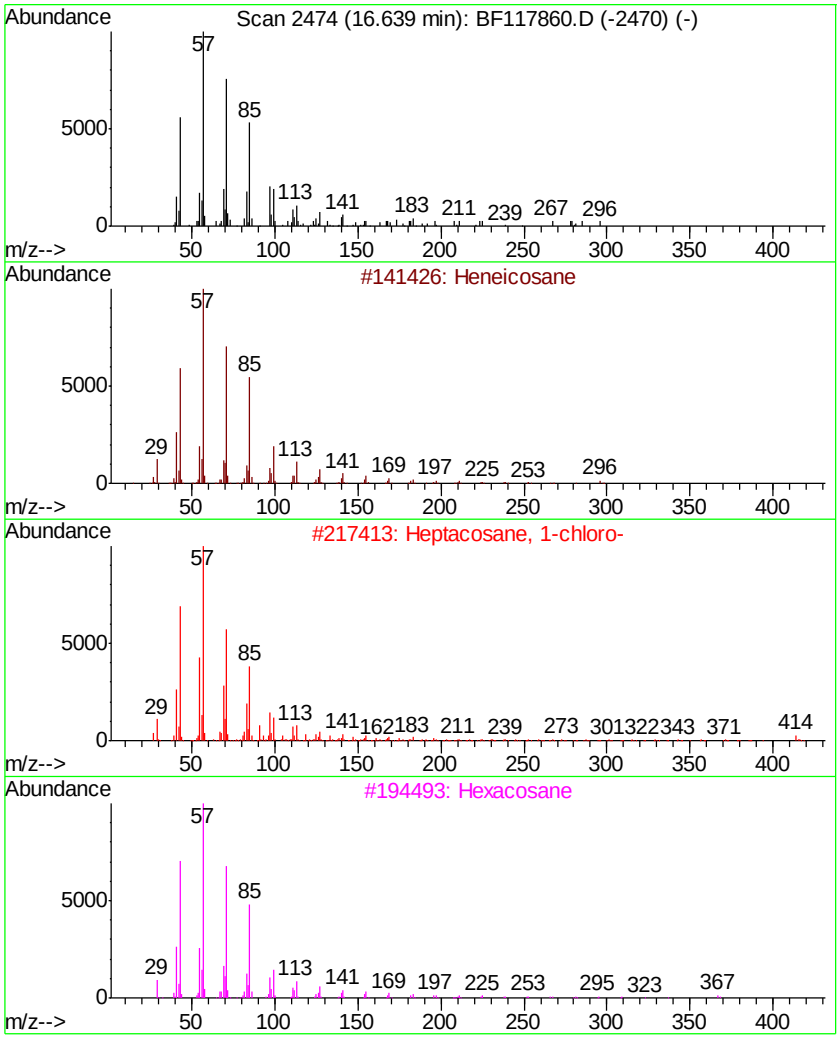
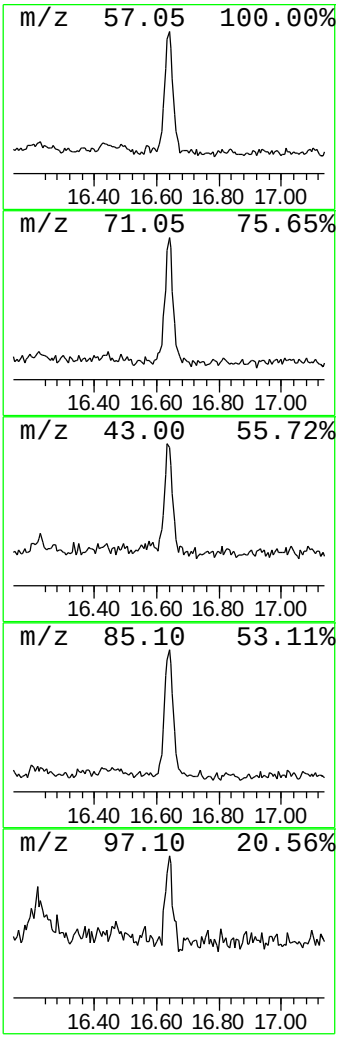
Peak Number 12 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.64	2.01 ng	145281	Perylene-d12	15.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	90
3	Hexacosane	366	C26H54	000630-01-3	87
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
5	Hentriacontane	437	C31H64	000630-04-6	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111919\
Data File : BF117860.D
Acq On : 19 Nov 2019 15:36
Operator : JU
Sample : K5865-17
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
2-(4-6)

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...	2.19	15.6	ng	971024	1	6.92	1248770	20.0
2-Pentanone, 4-hy...	5.13	12.1	ng	752182	1	6.92	1248770	20.0
unknown6.68	6.68	68.2	ng	4256160	1	6.92	1248770	20.0
Oxalic acid, isob...	13.95	4.3	ng	418500	5	14.10	1927720	20.0
Heptadecane	14.57	2.1	ng	206364	5	14.10	1927720	20.0
Octadecane	14.89	3.0	ng	218387	6	15.61	1445400	20.0
Nonadecane	15.24	3.2	ng	229429	6	15.61	1445400	20.0
Benzo[e]pyrene	15.54	2.0	ng	148107	6	15.61	1445400	20.0
Decane, 3,8-dimet...	16.10	3.0	ng	215552	6	15.61	1445400	20.0
Heneicosane	16.64	2.0	ng	145281	6	15.61	1445400	20.0