LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099446.D
Acq On : 13 Oct 2017 18:21
Operator : SJ/JU
Sample : I5713-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-18

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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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	2.134	3	8	16	rVB	175479	234546	8.27%	1.195%
2	5.075	505	508	522	rVB	167849	192656	6.79%	0.982%
3	5.475	572	576	593	rBV	1412386	1292989	45.59%	6.589%
4	6.481	744	747	757	rBV	824193	790365	27.87%	4.028%
5	6.622	767	771	775	rBV	2220224	2214103	78.06%	11.283%
6	6.851	807	810	818	rBV	674408	549695	19.38%	2.801%
7	7.010	833	837	840	rBV	2400358	2147589	75.72%	10.944%
8	7.422	902	907	910	rBV	1687995	1652488	58.26%	8.421%
9	8.133	1024	1028	1034	rBV	862610	721436	25.44%	3.676%
10	8.798	1139	1141	1144	rBV	71898	59304	2.09%	0.302%
11	8.945	1160	1166	1169	rBV4	32992	43889	1.55%	0.224%
12	9.210	1206	1211	1214	rBV	3182097	2836247	100.00%	14.453%
13	9.386	1237	1241	1249	rVB6	22591	43563	1.54%	0.222%
14	9.551	1264	1269	1273	rBV5	26994	32409	1.14%	0.165%
15	9.598	1274	1277	1280	rBV	123692	101148	3.57%	0.515%
16	9.886	1318	1326	1331	rBV	813084	739591	26.08%	3.769%
17	10.092	1358	1361	1365	rVB	34982	31526	1.11%	0.161%
18	10.251	1385	1388	1390	rBV4	26887	31730	1.12%	0.162%
19	10.433	1416	1419	1424	rBV2	26256	31356	1.11%	0.160%
20	10.680	1457	1461	1467	rBV	1422932	1294738	45.65%	6.598%
21	11.374	1575	1579	1583	rBV	660725	577693	20.37%	2.944%
22	11.586	1612	1615	1622	rBV4	42933	49171	1.73%	0.251%
23	11.892	1664	1667	1672	rBV2	36494	36622	1.29%	0.187%
24	12.404	1751	1754	1761	rBV	209246	211846	7.47%	1.080%
25	12.463	1761	1764	1769	rVB3	34276	38789	1.37%	0.198%
26	12.957	1844	1848	1852	rBV	1882907	1846276	65.10%	9.408%
27	13.151	1879	1881	1888	rBV2	38289	48824	1.72%	0.249%
28	13.398	1920	1923	1926	rVB	71015	61748	2.18%	0.315%
29	13.839	1995	1998	2004	rBV3	51107	55846	1.97%	0.285%
30	13.980	2019	2022	2025	rBV	60776	52479	1.85%	0.267%
31	14.015	2025	2028	2034	rVV	573242	514733	18.15%	2.623%
32	15.492	2273	2279	2284	rBV	470096	599811	21.15%	3.057%
33	15.909	2346	2350	2357	rVB2	51213	77564	2.73%	0.395%
34	16.409	2431	2435	2442	rVB2	63864	104038	3.67%	0.530%

LSC Area Percent Report

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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-18

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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.003	2529	2536	2543	rVB2	49175	108544	3.83%	0.553%
36	17.697	2648	2654	2664	rVB2	47527	116799	4.12%	0.595%
37	18.515	2787	2793	2802	rBV4	26997	81798	2.88%	0.417%

Sum of corrected areas: 19623949

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099446.D
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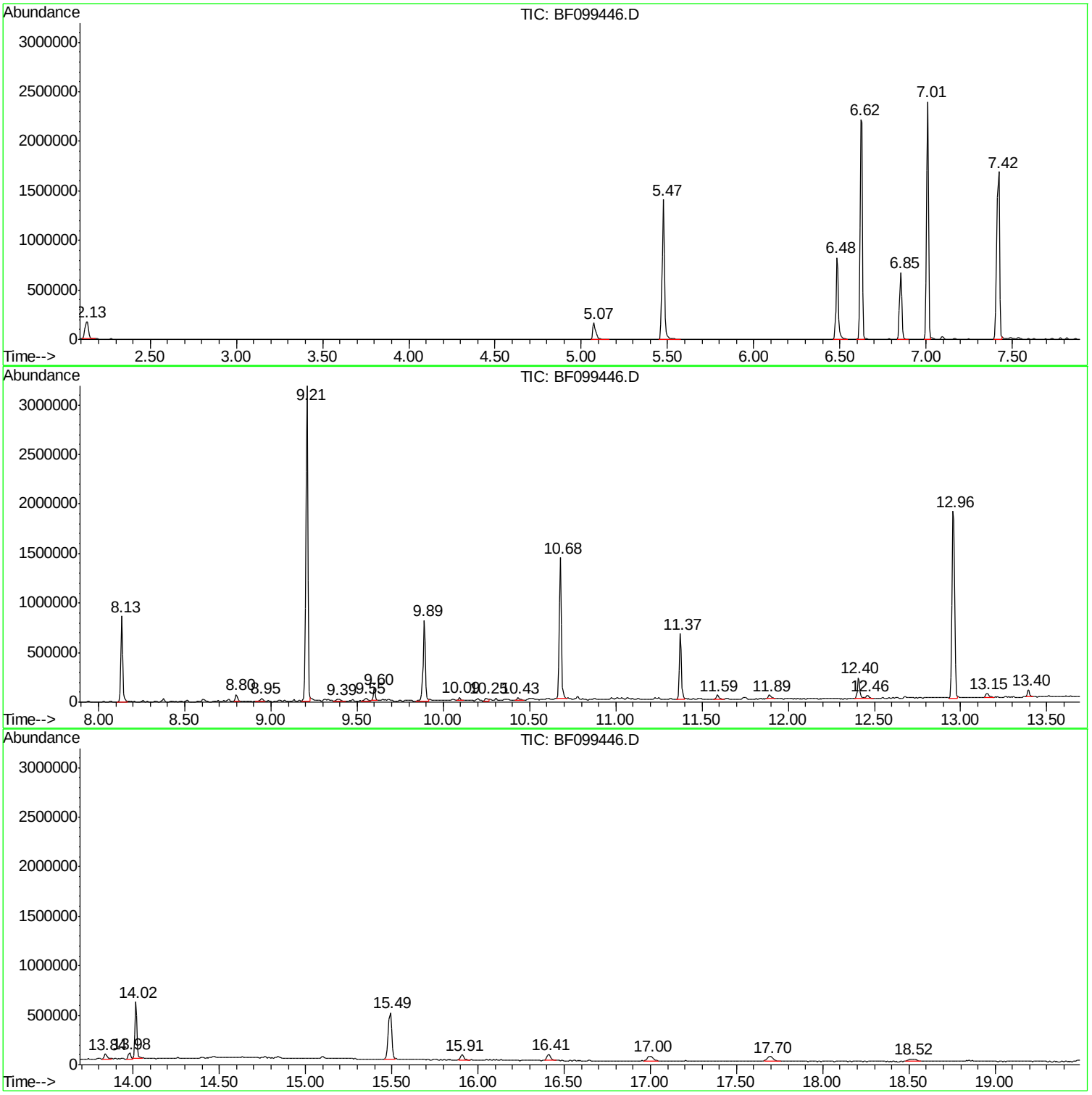
Operator : SJ/JU
Sample : I5713-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099446.D
Acq On : 13 Oct 2017 18:21
Operator : SJ/JU
Sample : I5713-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

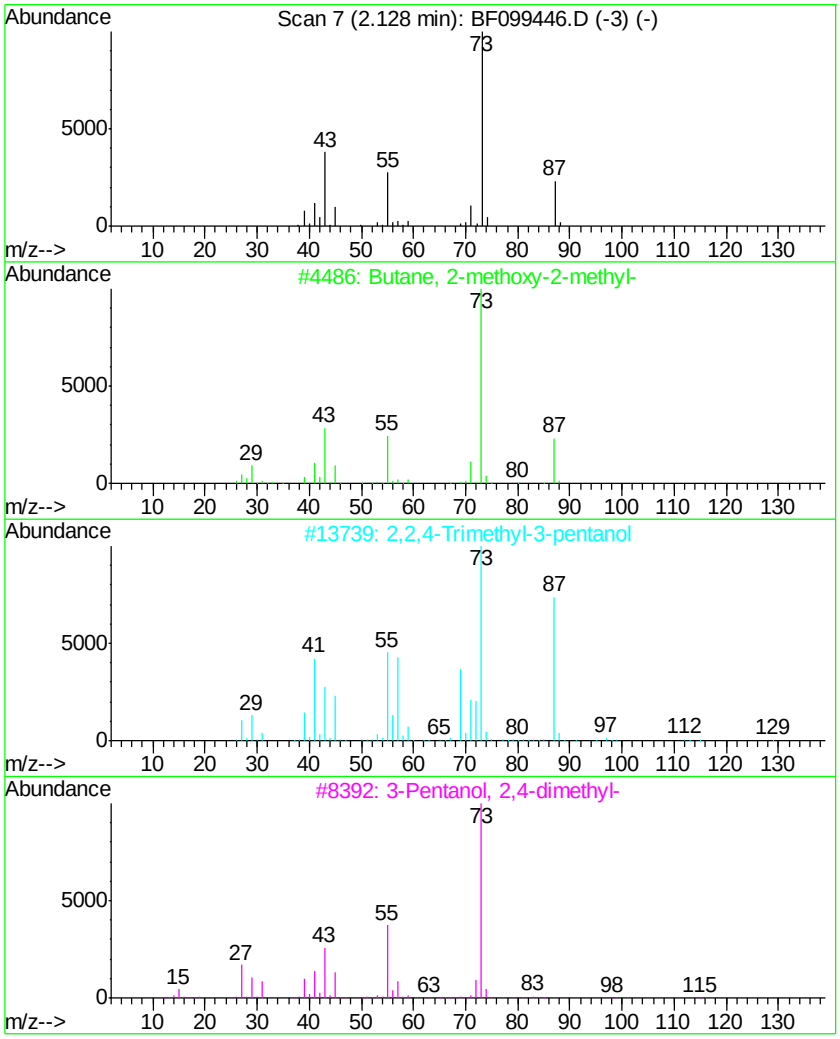
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

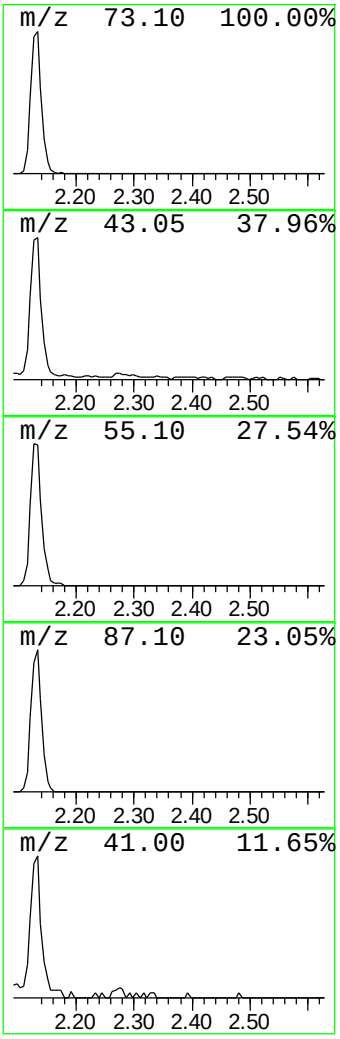
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	8.53 ng	234546	1,4-Dichlorobenzene-d4	6.85

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	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10





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Operator : SJ/JU
Sample : I5713-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

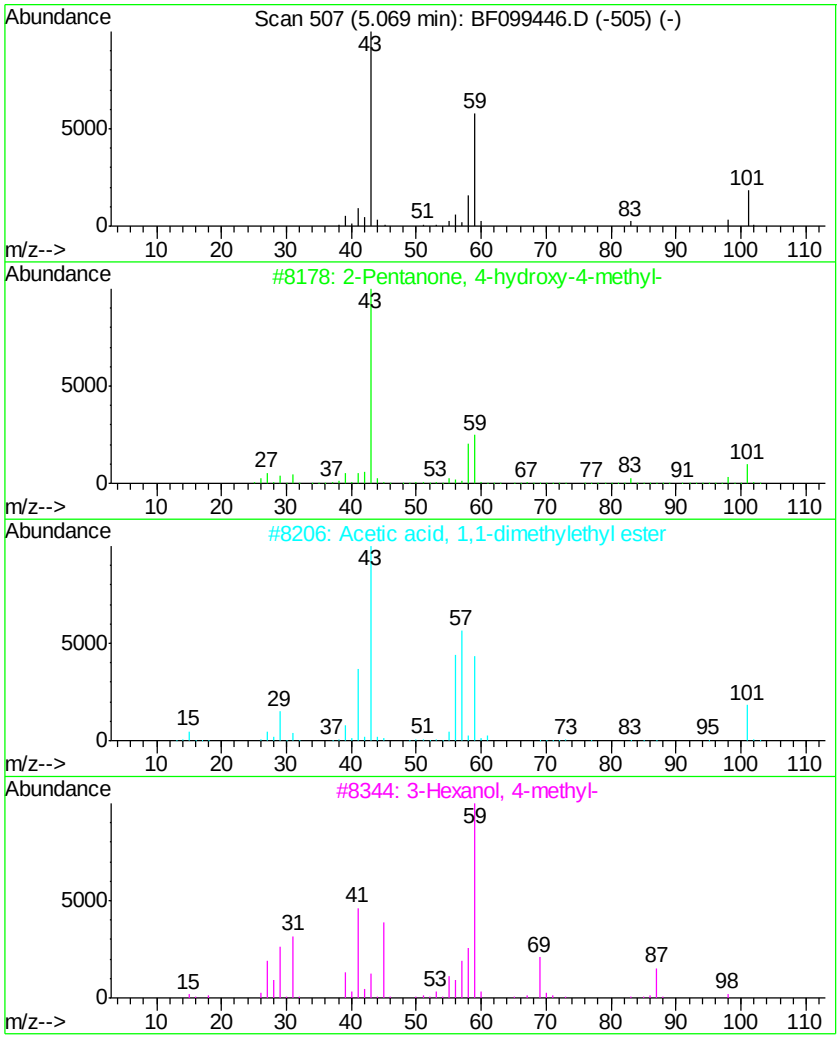
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

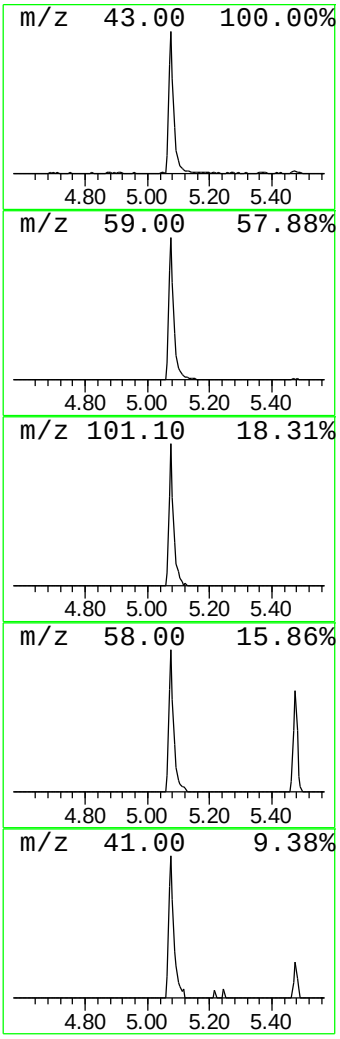
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	7.01 ng	192656	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099446.D
Acq On : 13 Oct 2017 18:21
Operator : SJ/JU
Sample : I5713-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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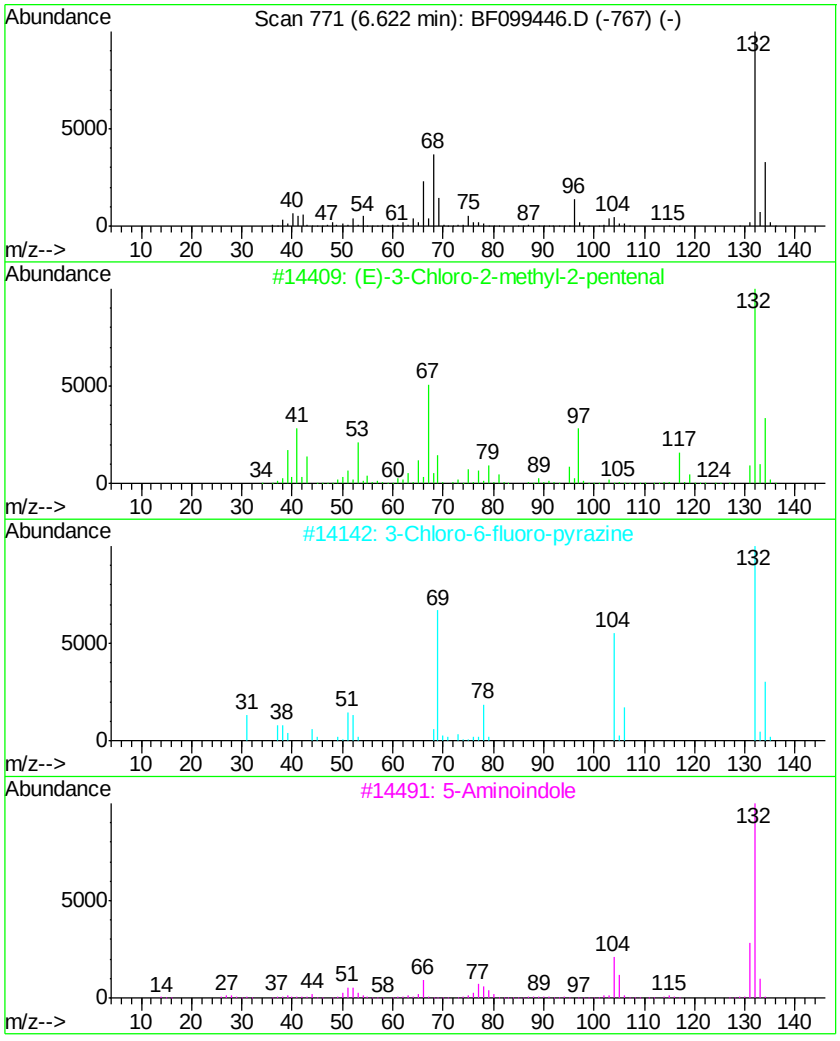
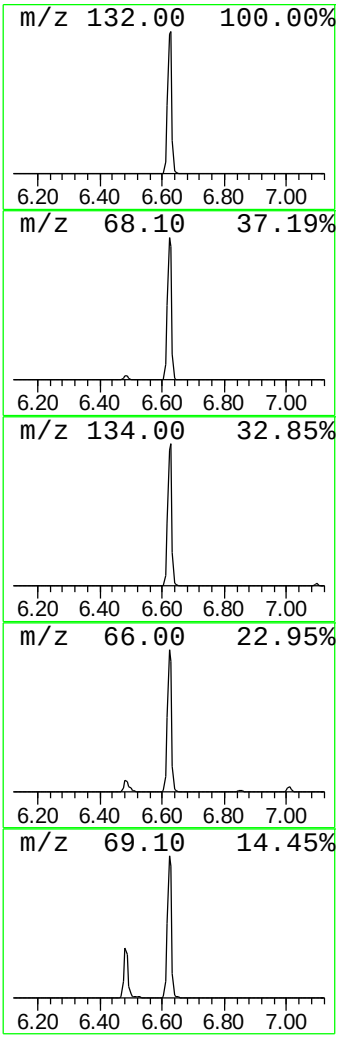
Peak Number 3 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	80.56 ng	2214100	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099446.D
Acq On : 13 Oct 2017 18:21
Operator : SJ/JU
Sample : I5713-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

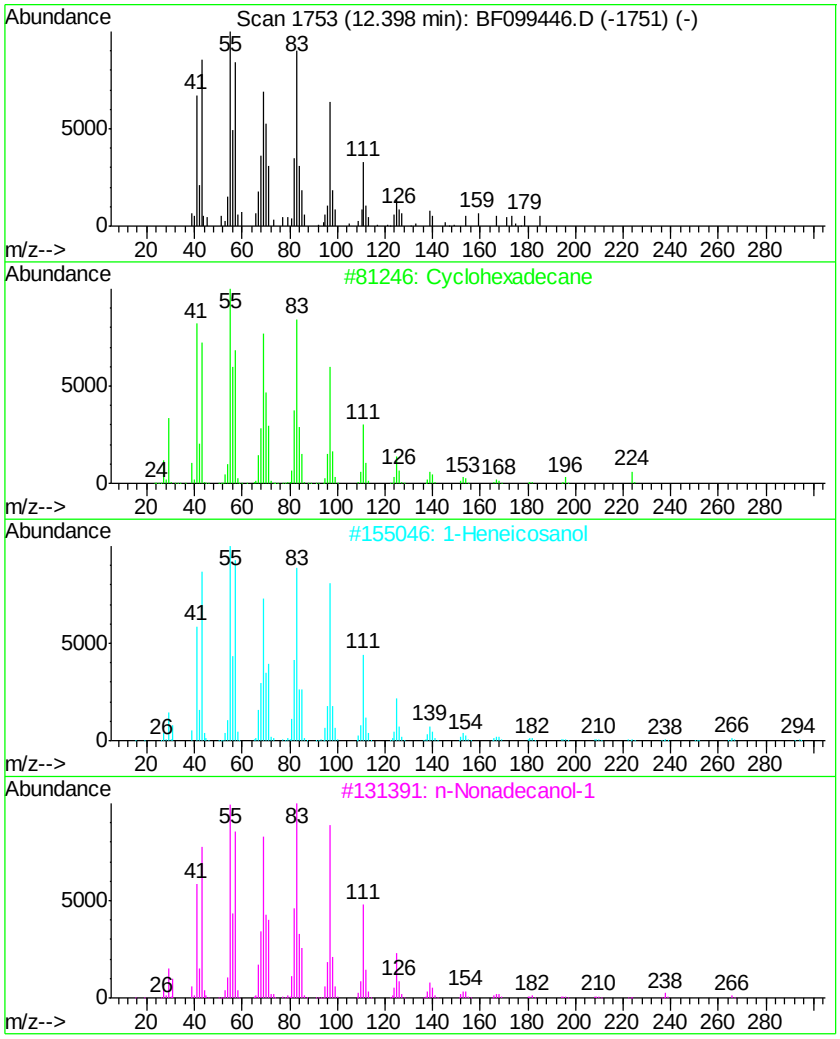
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

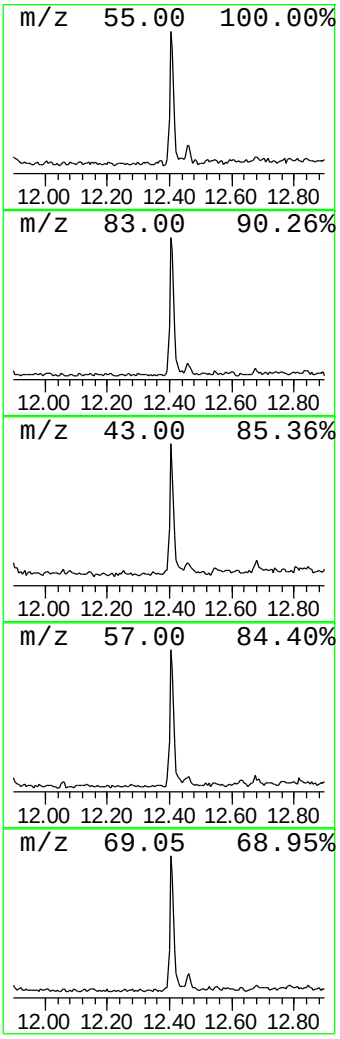
****

Peak Number 5 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.40	7.33 ng	211846	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	99
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4	1-Hexadecanol	242	C16H34O	036653-82-4	94
5	Dichloroacetic acid, 4-hexadecyl...	352	C18H34Cl2O2	1000282-98-1	94





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Sample : I5713-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

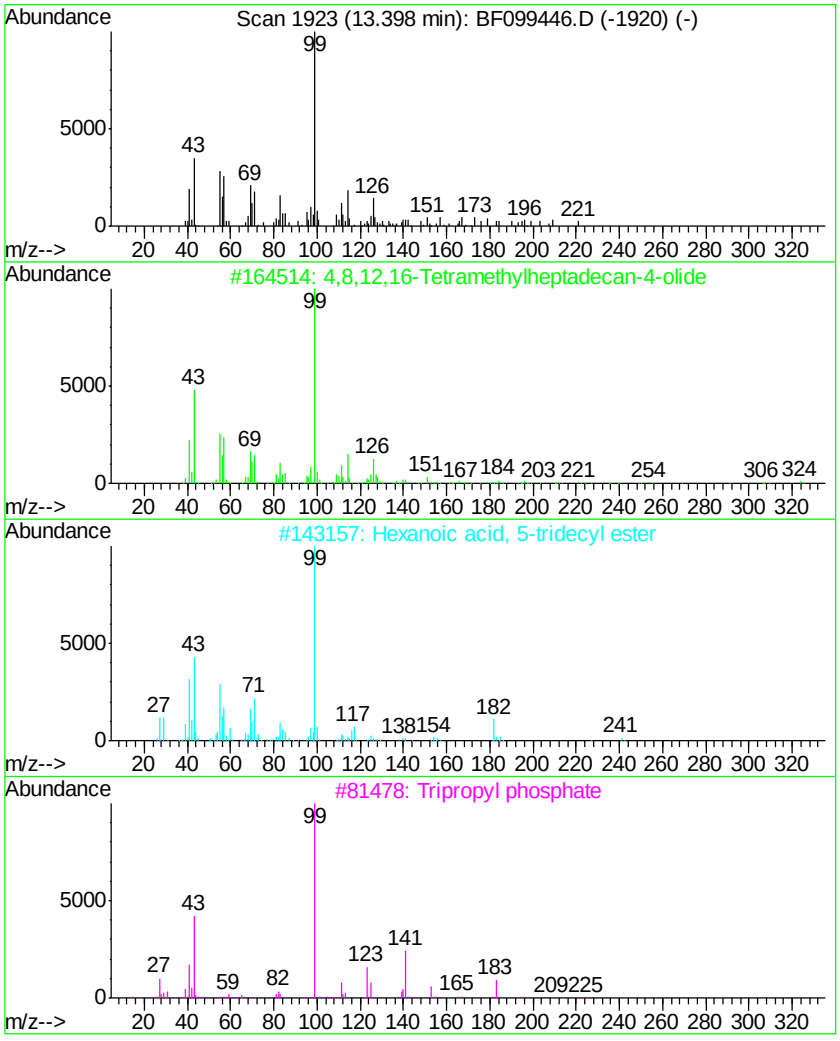
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

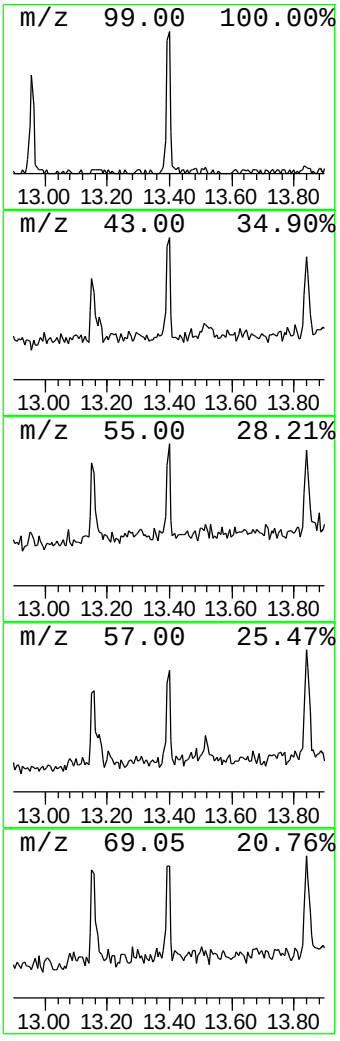
****

Peak Number 6 4,8,12,16-Tetramethylheptad... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.40	2.40 ng	61748	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,8,12,16-Tetramethylheptadecan-...	324	C21H40O2	096168-15-9	90
2	Hexanoic acid, 5-tridecyl ester	298	C19H38O2	1000279-29-4	53
3	Tripropyl phosphate	224	C9H21O4P	000513-08-6	50
4	Hexanoic acid, 4-tetradecyl ester	312	C20H40O2	1000279-29-8	50
5	Hexanamide, N-allyl-	155	C9H17NO	1000340-13-9	50





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Sample : I5713-10
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Instrument : BNA_F
ClientSampleId : MW-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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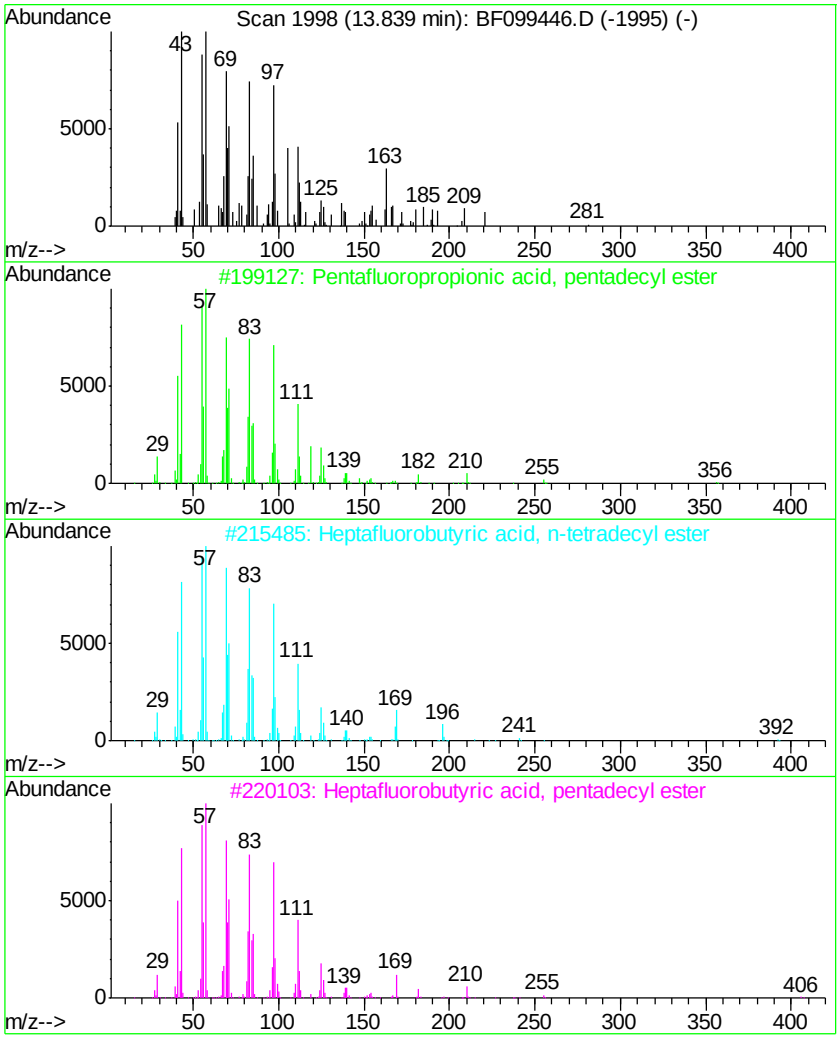
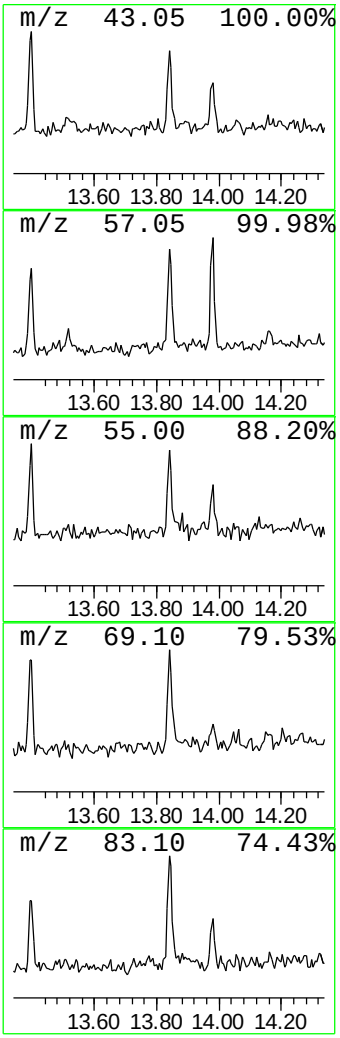
Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	2.17 ng	55846	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	90
2	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	90
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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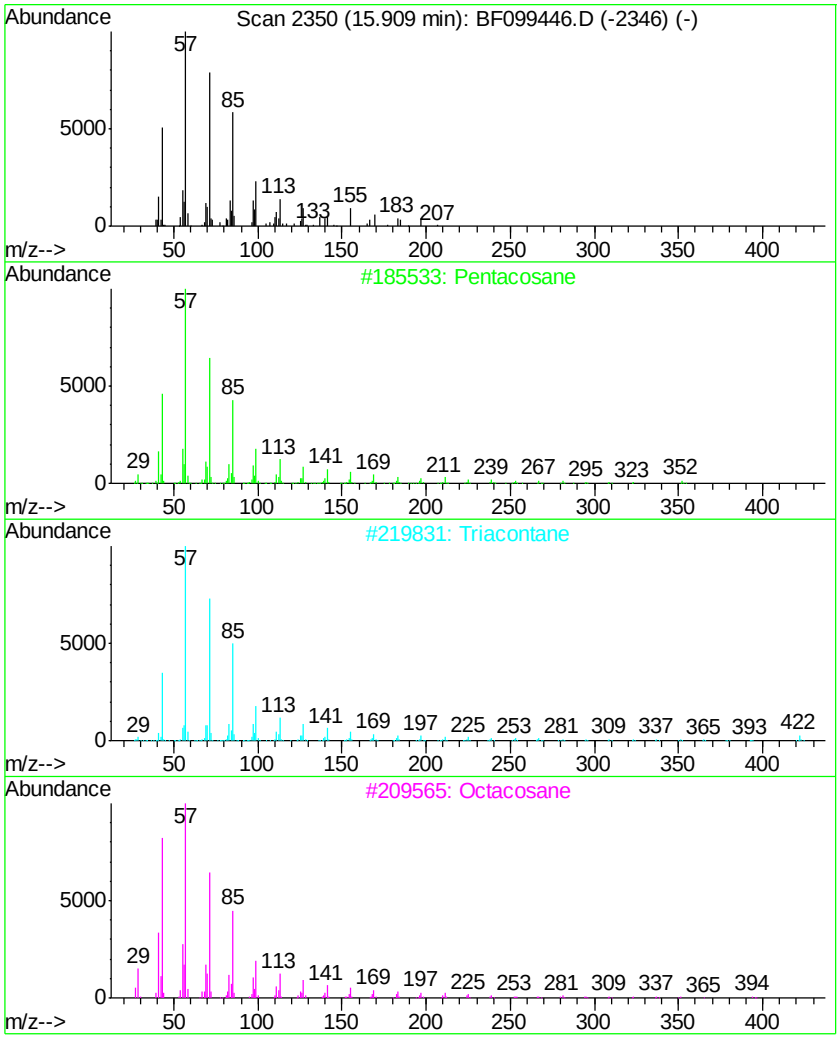
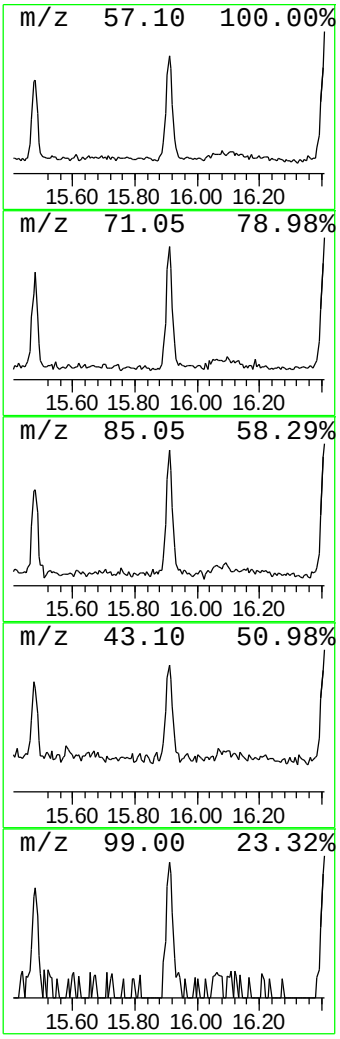
Peak Number 8 Pentacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.91	2.59 ng	77564	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	91
2	Triacontane	422	C30H62	000638-68-6	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Hexacosane	366	C26H54	000630-01-3	90
5	Heneicosane	296	C21H44	000629-94-7	90





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099446.D
Acq On : 13 Oct 2017 18:21
Operator : SJ/JU
Sample : I5713-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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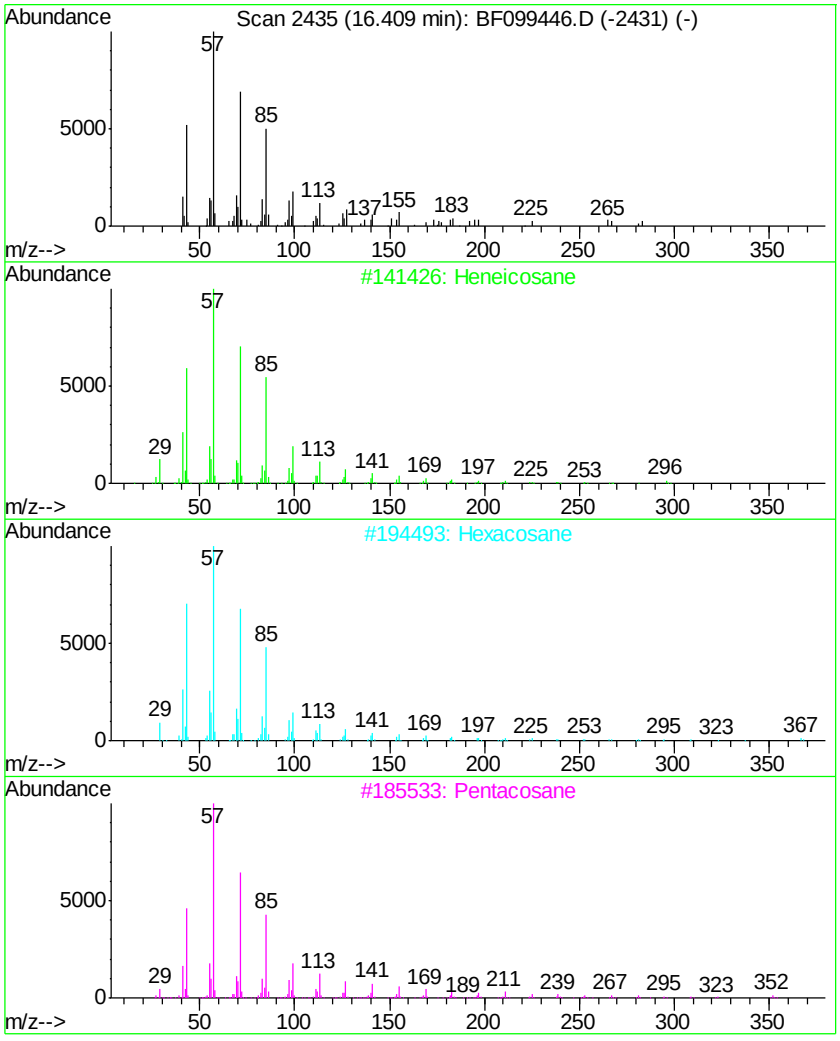
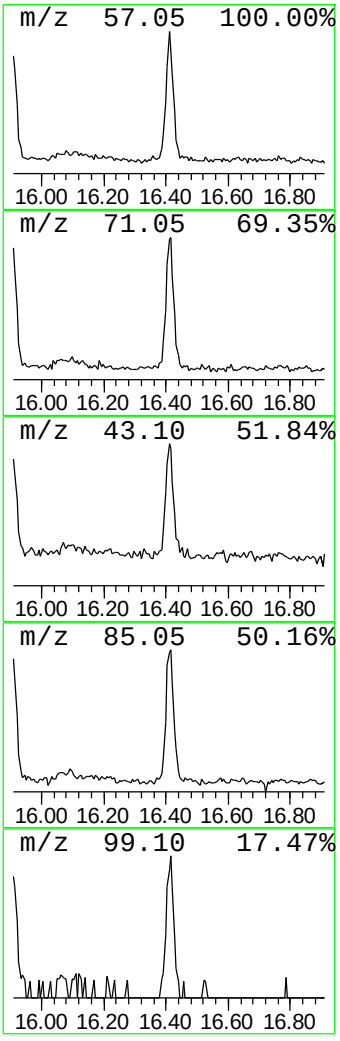
Peak Number 9 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.41	3.47 ng	104038	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Hexacosane	366	C26H54	000630-01-3	90
3	Pentacosane	352	C25H52	000629-99-2	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Hentriacontane	437	C31H64	000630-04-6	90





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Data File : BF099446.D
Acq On : 13 Oct 2017 18:21
Operator : SJ/JU
Sample : I5713-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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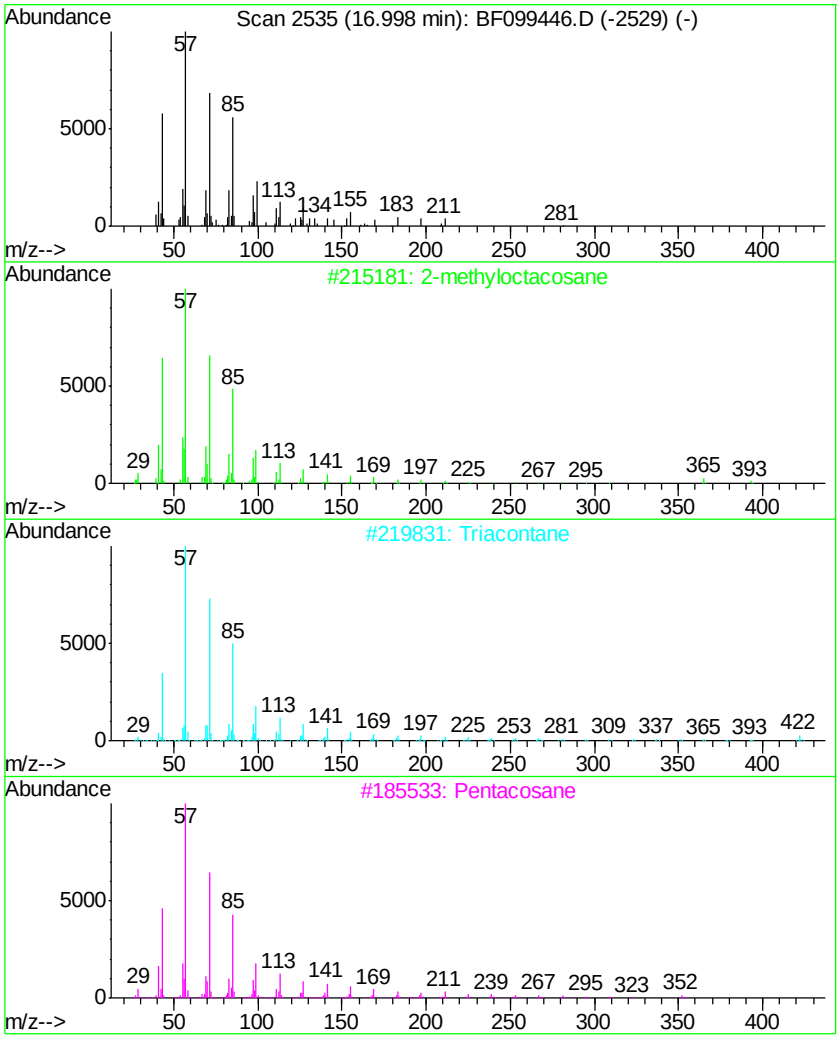
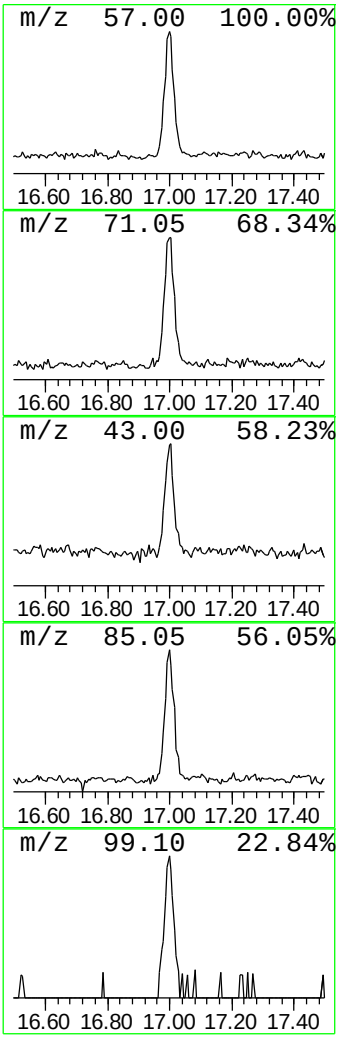
Peak Number 10 2-methyloctacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.00	3.62 ng	108544	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	87
2	Triacontane	422	C30H62	000638-68-6	87
3	Pentacosane	352	C25H52	000629-99-2	86
4	Tetratetracontane	619	C44H90	007098-22-8	80
5	Octacosane	394	C28H58	000630-02-4	72





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Operator : SJ/JU
Sample : I5713-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-18

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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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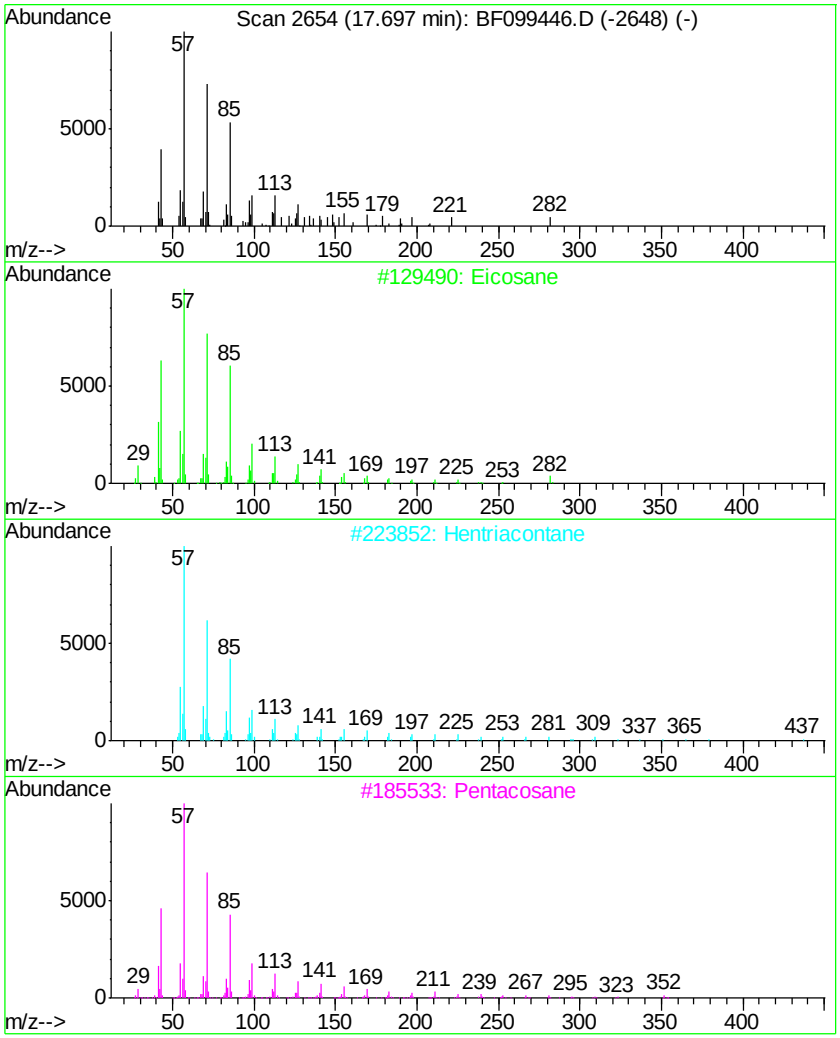
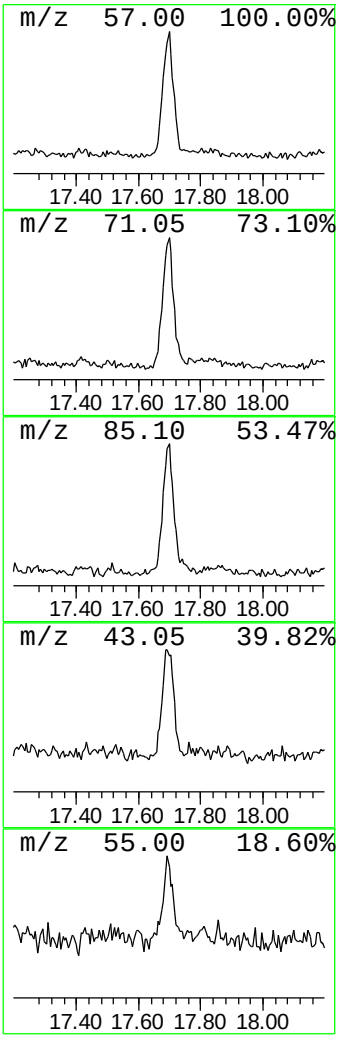
Peak Number 11 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.70	3.89 ng	116799	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Hentriacontane	437	C31H64	000630-04-6	87
3	Pentacosane	352	C25H52	000629-99-2	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Triacontane	422	C30H62	000638-68-6	86





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Data File : BF099446.D
Acq On : 13 Oct 2017 18:21
Operator : SJ/JU
Sample : I5713-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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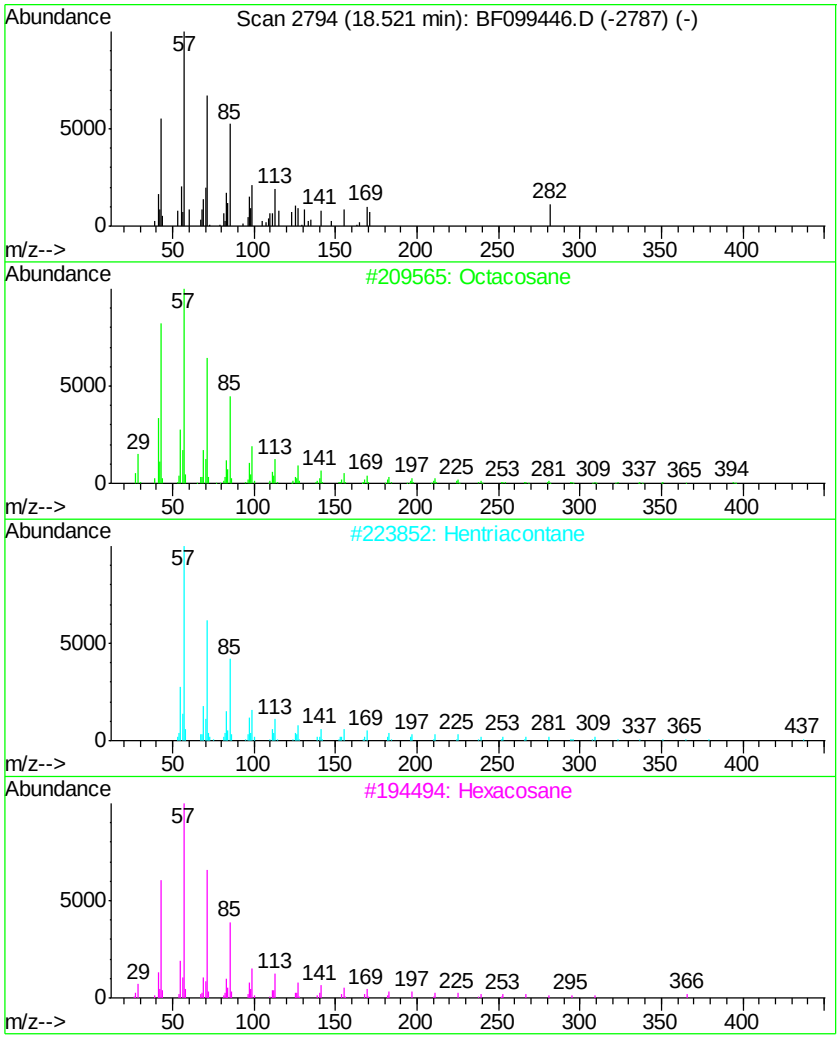
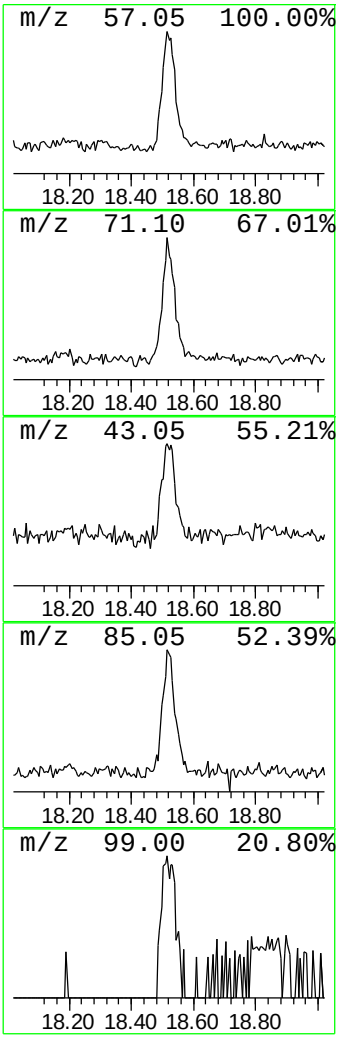
Peak Number 12 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.52	2.73 ng	81798	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hentriacontane	437	C31H64	000630-04-6	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Pentacosane	352	C25H52	000629-99-2	90
5	Triacontane	422	C30H62	000638-68-6	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099446.D
Acq On : 13 Oct 2017 18:21
Operator : SJ/JU
Sample : I5713-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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...	2.13	8.5	ng	234546	1	6.85	549695	20.0
2-Pentanone, 4-hy...	5.07	7.0	ng	192656	1	6.85	549695	20.0
unknown6.62	6.62	80.6	ng	2214100	1	6.85	549695	20.0
Cyclohexadecane	12.40	7.3	ng	211846	4	11.37	577693	20.0
4,8,12,16-Tetrame...	13.40	2.4	ng	61748	5	14.02	514733	20.0
Pentafluoropropio...	13.84	2.2	ng	55846	5	14.02	514733	20.0
Pentacosane	15.91	2.6	ng	77564	6	15.49	599811	20.0
Heneicosane	16.41	3.5	ng	104038	6	15.49	599811	20.0
2-methyloctacosane	17.00	3.6	ng	108544	6	15.49	599811	20.0
Eicosane	17.70	3.9	ng	116799	6	15.49	599811	20.0
Octacosane	18.52	2.7	ng	81798	6	15.49	599811	20.0