LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041618\
Data File : BF104558.D
Acq On : 17 Apr 2018 2:38
Operator : JU/SJ
Sample : J2360-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NAA-WS-003

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-BF040618.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	5.022	495	499	510	rVB	111861	154022	4.79%	0.553%
2	5.428	563	568	572	rBV	2747327	2920842	90.82%	10.479%
3	6.057	672	675	682	rVB	73204	90985	2.83%	0.326%
4	6.451	736	742	746	rBV	2666671	2976024	92.53%	10.677%
5	6.581	759	764	767	rBV	3171418	2963784	92.15%	10.633%
6	6.810	799	803	806	rBV	1152730	902064	28.05%	3.236%
7	6.969	825	830	833	rBV	2558238	2410194	74.94%	8.647%
8	7.375	894	899	902	rBV	2036315	1873715	58.26%	6.722%
9	8.092	1017	1021	1024	rBV	1439992	1146704	35.65%	4.114%
10	9.169	1199	1204	1207	rBV	3437575	3216115	100.00%	11.538%
11	9.563	1267	1271	1274	rBV	360401	300557	9.35%	1.078%
12	9.775	1303	1307	1310	rBV	119538	90141	2.80%	0.323%
13	9.851	1316	1320	1328	rVB	1270183	1141772	35.50%	4.096%
14	10.275	1389	1392	1395	rVB	143912	107993	3.36%	0.387%
15	10.498	1423	1430	1432	rBV	34450	44332	1.38%	0.159%
16	10.639	1451	1454	1465	rVB	1540079	1450616	45.10%	5.204%
17	10.751	1470	1473	1483	rVB	113077	118394	3.68%	0.425%
18	11.198	1546	1549	1551	rBV	51547	39301	1.22%	0.141%
19	11.339	1569	1573	1577	rBV	1091914	892668	27.76%	3.203%
20	12.745	1808	1812	1815	rVB	407637	326961	10.17%	1.173%
21	12.821	1822	1825	1828	rVB	66342	56969	1.77%	0.204%
22	12.927	1839	1843	1846	rBV	2427737	2202415	68.48%	7.902%
23	13.451	1928	1932	1936	rBV	294361	236934	7.37%	0.850%
24	13.498	1936	1940	1942	rBV	43751	38371	1.19%	0.138%
25	13.821	1992	1995	2006	rBV2	140627	156576	4.87%	0.562%
26	13.986	2019	2023	2026	rBV	927847	799255	24.85%	2.867%
27	14.145	2046	2050	2055	rBV	66176	66372	2.06%	0.238%
28	14.451	2098	2102	2106	rBV	72767	67686	2.10%	0.243%
29	14.757	2150	2154	2159	rVB	88553	88673	2.76%	0.318%
30	14.827	2163	2166	2169	rVB	47092	44219	1.37%	0.159%
31	15.086	2206	2210	2215	rBV	67855	83913	2.61%	0.301%
32	15.451	2266	2272	2283	rBV	497928	699622	21.75%	2.510%
33	15.898	2344	2348	2353	rBV2	45844	65532	2.04%	0.235%
34	16.398	2429	2433	2438	rBV2	40365	63526	1.98%	0.228%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041618\
Data File : BF104558.D
Acq On : 17 Apr 2018 2:38
Operator : JU/SJ
Sample : J2360-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NAA-WS-003

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-BF040618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.992	2530	2534	2539	rVB3	21163	35980	1.12%	0.129%

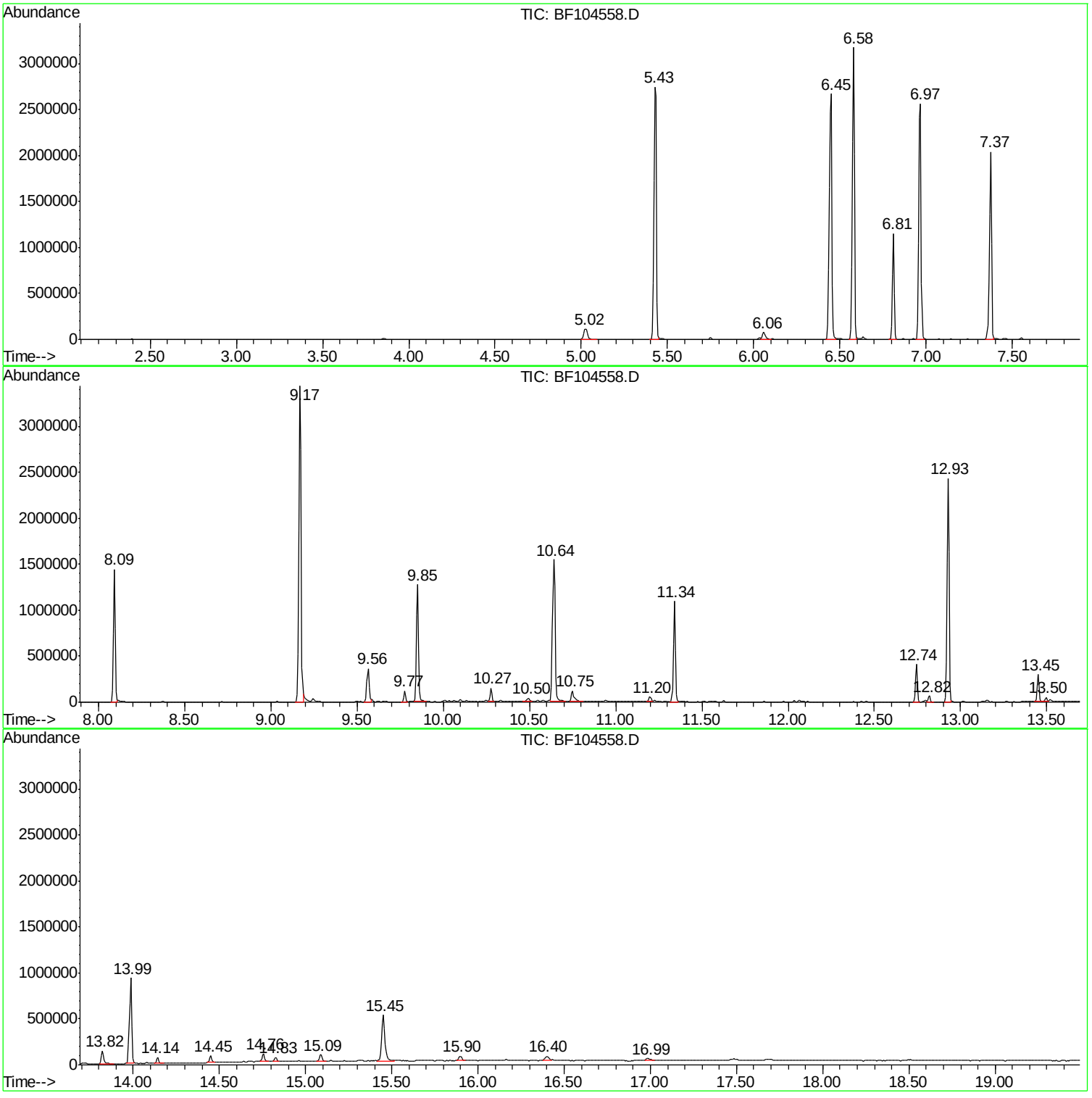
Sum of corrected areas: 27873227

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041618\
Data File : BF104558.D
Acq On : 17 Apr 2018 2:38
Operator : JU/SJ
Sample : J2360-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NAA-WS-003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF041618\
Data File : BF104558.D
Acq On : 17 Apr 2018 2:38
Operator : JU/SJ
Sample : J2360-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

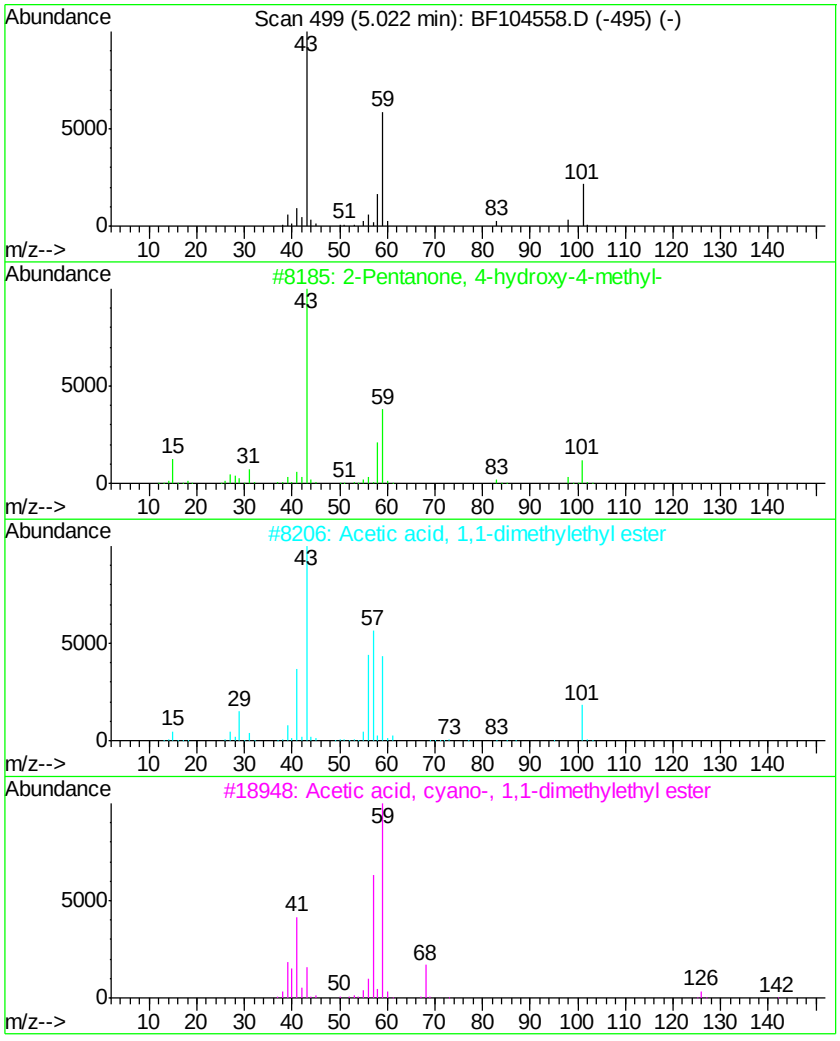
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

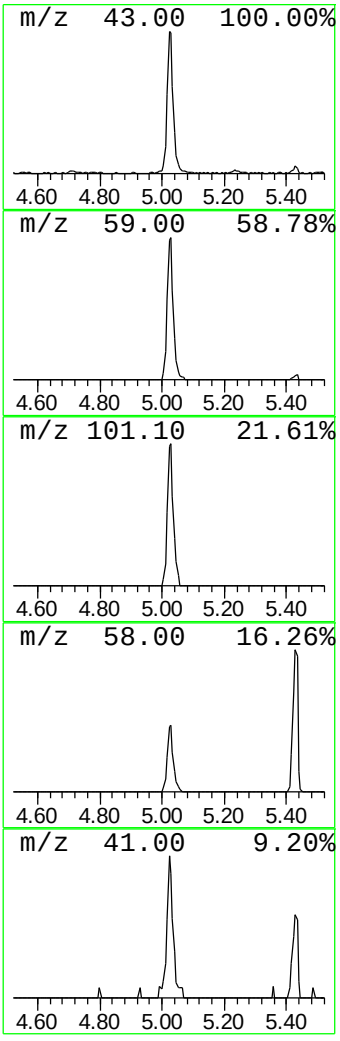
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	3.41 ng	154022	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041618\
Data File : BF104558.D
Acq On : 17 Apr 2018 2:38
Operator : JU/SJ
Sample : J2360-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NAA-WS-003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

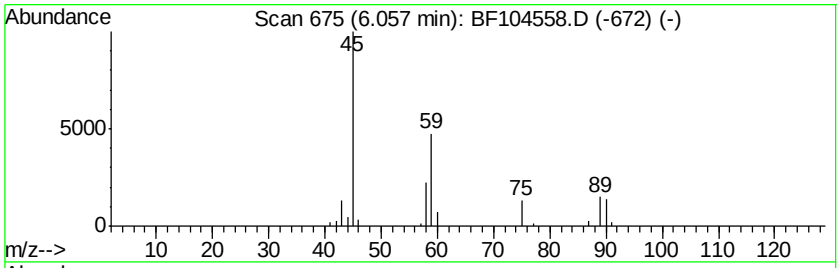
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

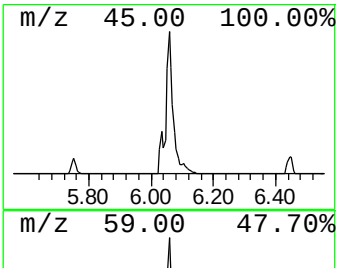
****

Peak Number 2 Ethanol, 2-(2-methoxyethoxy)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.06	2.02 ng	90985	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	83
2	Ethane, 1-methoxy-2-(methoxymeth...	120	C5H12O3	074498-88-7	64
3	Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	46
4	Ethane, 1,2-dimethoxy-	90	C4H10O2	000110-71-4	37
5	Hydrazine, (2-methoxyethyl)-	90	C3H10N2O	003044-15-3	37





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041618\
Data File : BF104558.D
Acq On : 17 Apr 2018 2:38
Operator : JU/SJ
Sample : J2360-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NAA-WS-003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

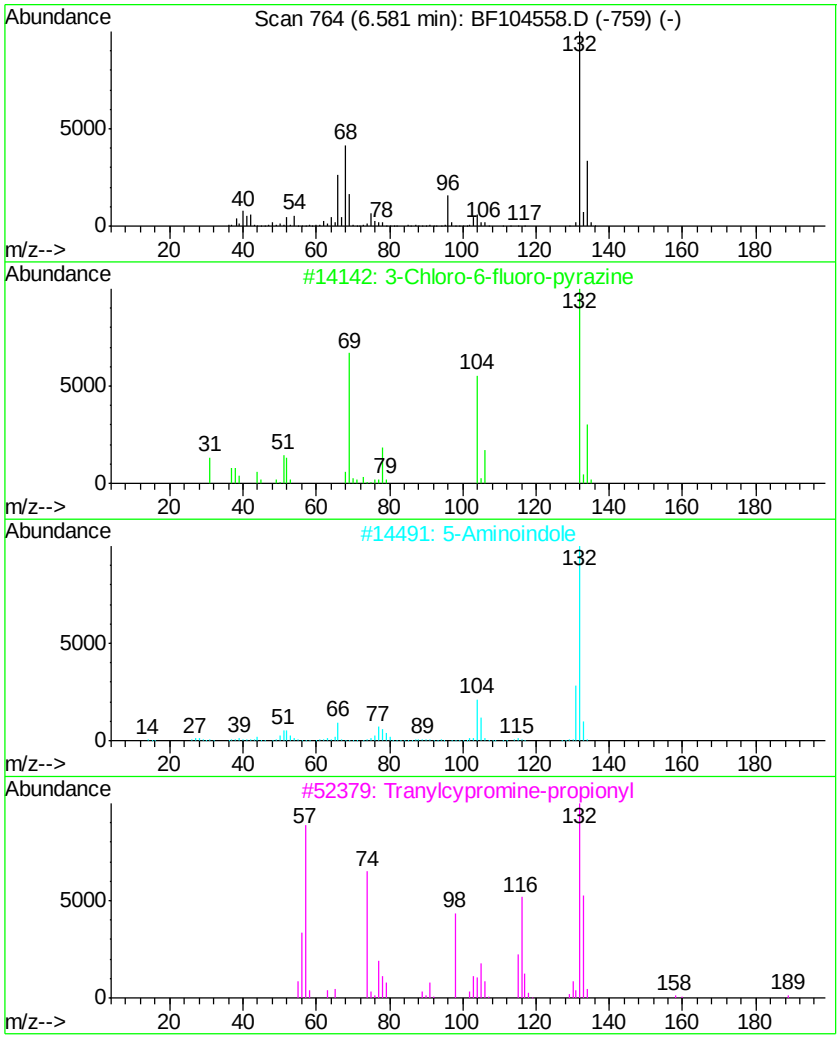
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

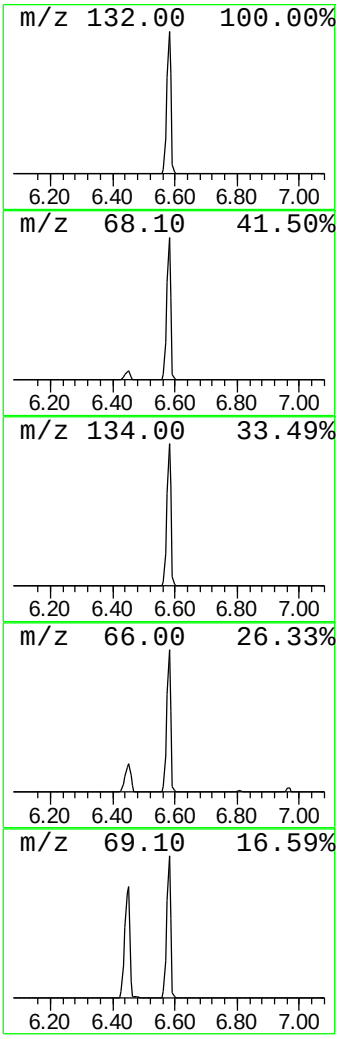
****

Peak Number 3 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	65.71 ng	2963780	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041618\
Data File : BF104558.D
Acq On : 17 Apr 2018 2:38
Operator : JU/SJ
Sample : J2360-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NAA-WS-003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

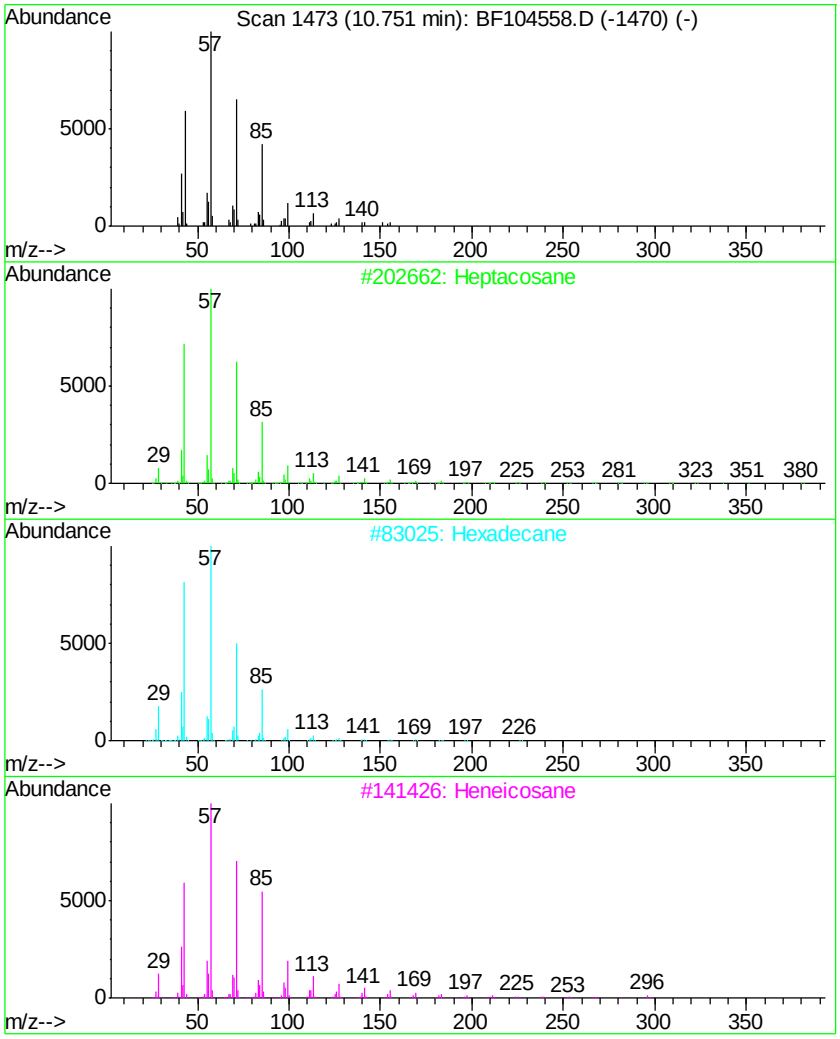
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

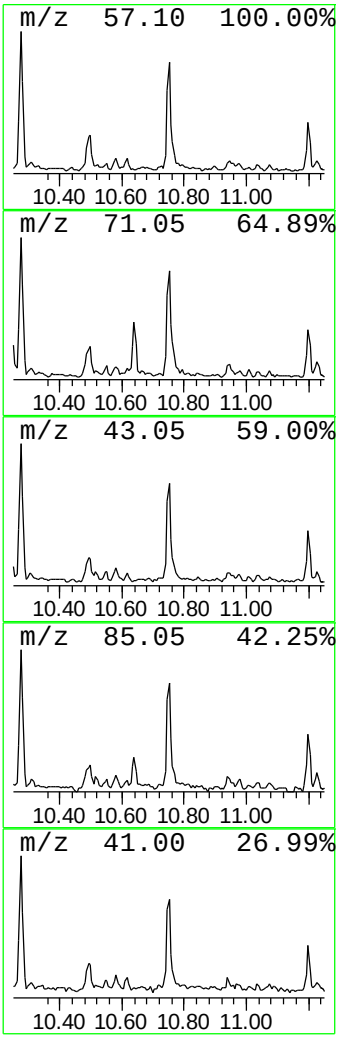
****

Peak Number 5 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	2.65 ng	118394	Phenanthrene-d10	11.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Octacosane	394	C28H58	000630-02-4	87
5	Nonadecane	268	C19H40	000629-92-5	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041618\
Data File : BF104558.D
Acq On : 17 Apr 2018 2:38
Operator : JU/SJ
Sample : J2360-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NAA-WS-003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

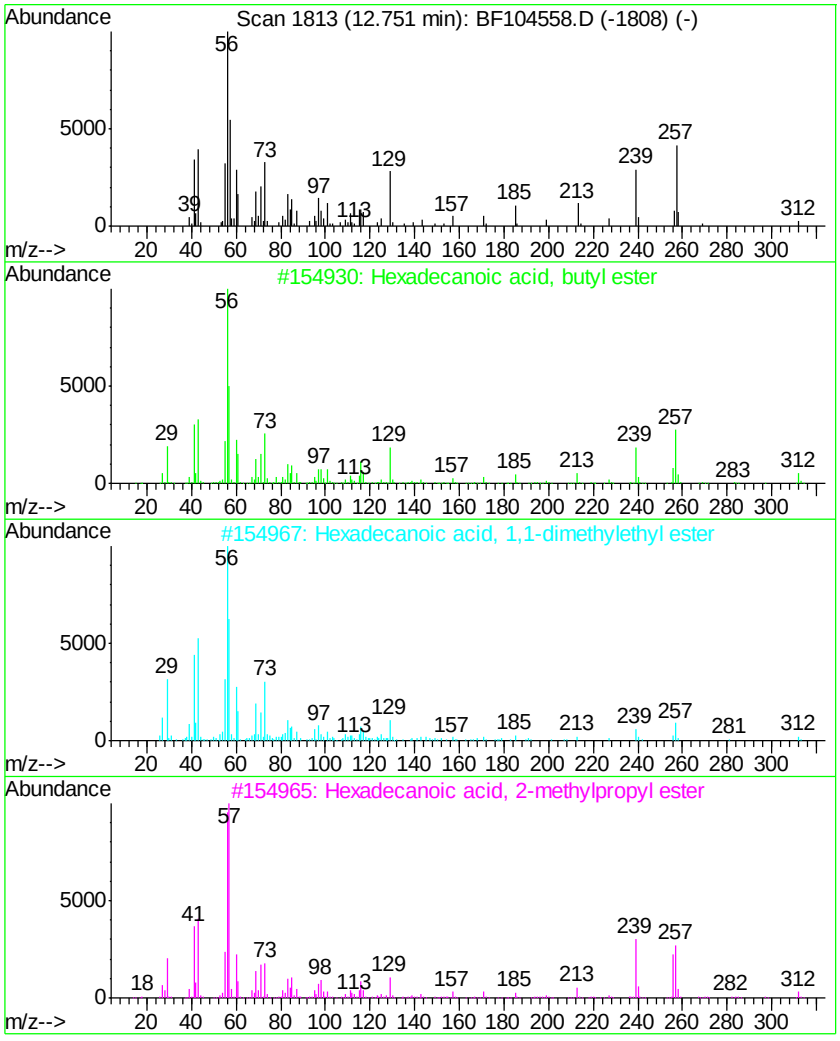
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

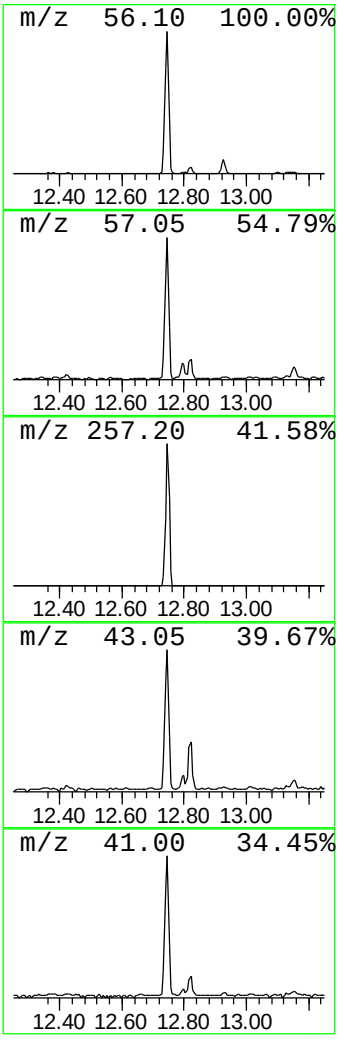
****

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.75	8.18 ng	326961	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	62
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	59
4	Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	45
5	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041618\
Data File : BF104558.D
Acq On : 17 Apr 2018 2:38
Operator : JU/SJ
Sample : J2360-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NAA-WS-003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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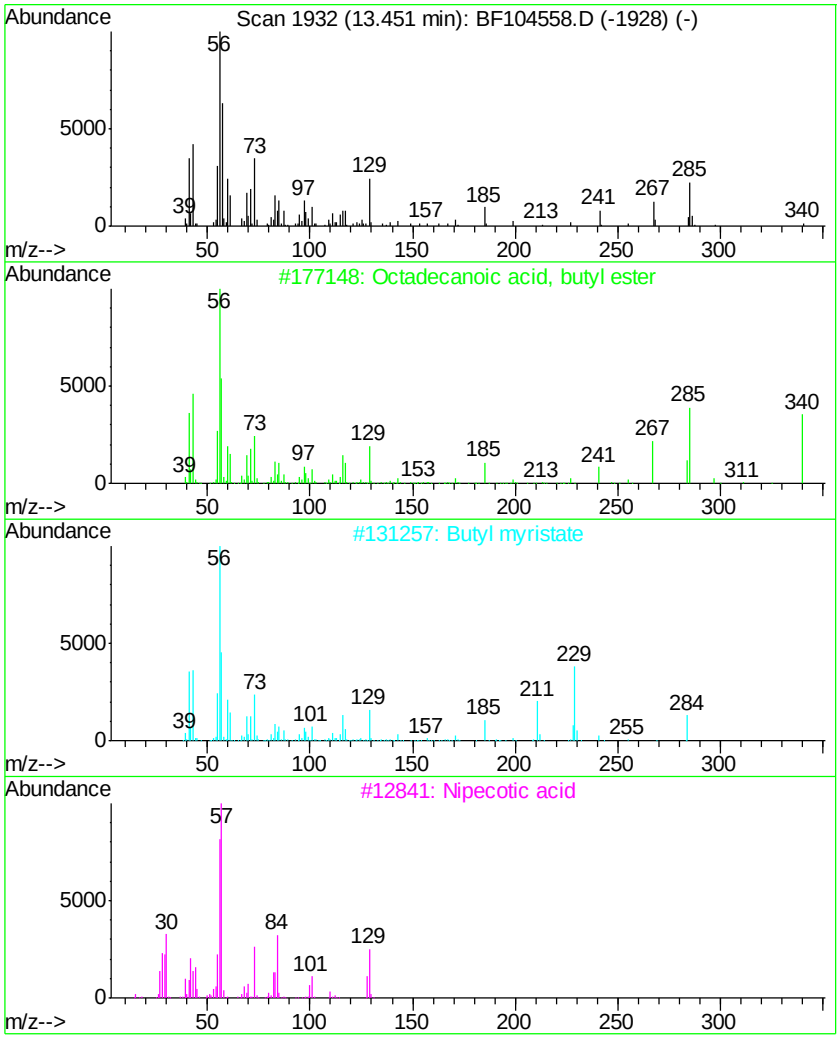
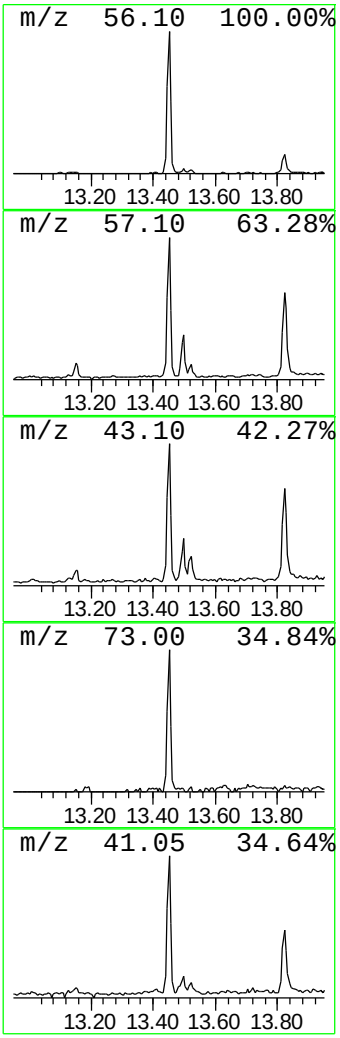
Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	5.93 ng	236934	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	93
2	Butyl myristate	284	C18H36O2	000110-36-1	64
3	Nipecotic acid	129	C6H11NO2	000498-95-3	47
4	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	38
5	Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041618\
Data File : BF104558.D
Acq On : 17 Apr 2018 2:38
Operator : JU/SJ
Sample : J2360-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NAA-WS-003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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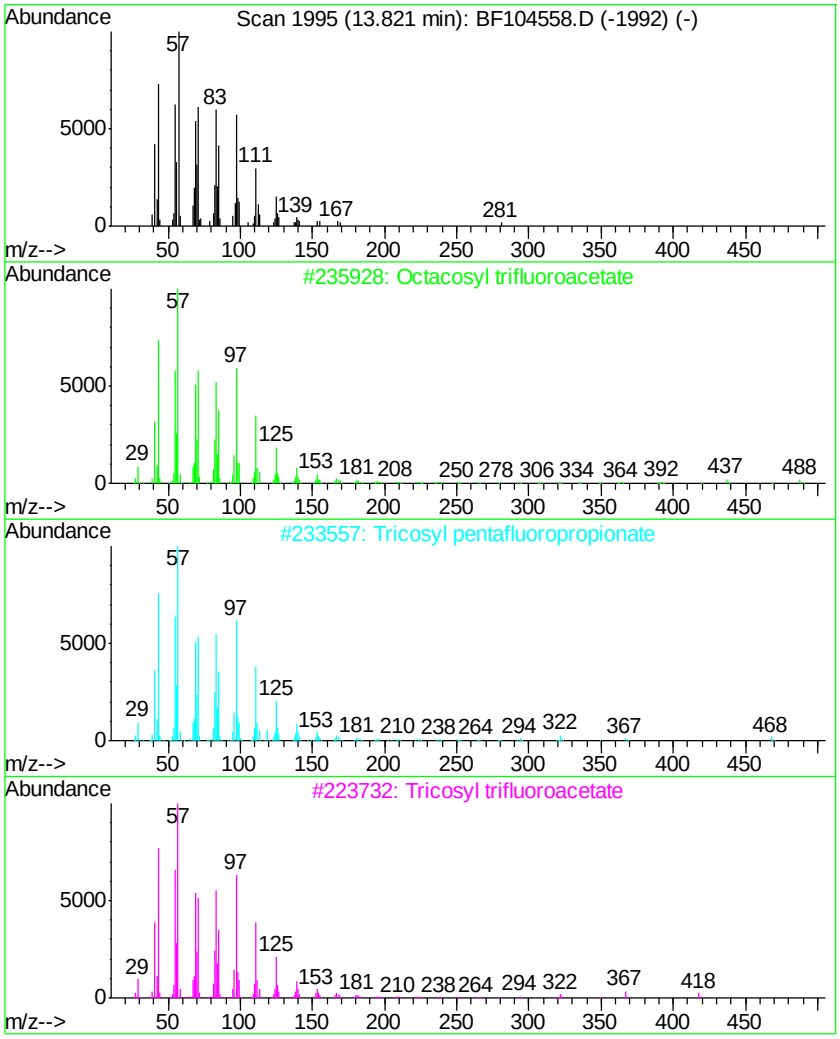
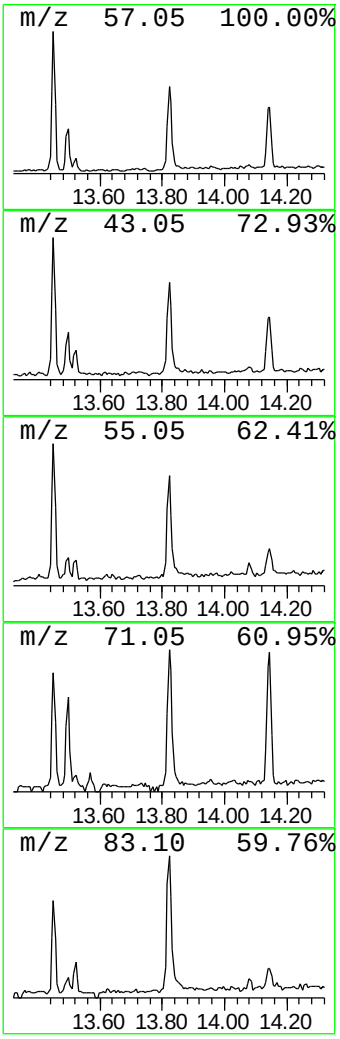
Peak Number 8 Octacosyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	3.92 ng	156576	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
2	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	91
3	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
4	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041618\
Data File : BF104558.D
Acq On : 17 Apr 2018 2:38
Operator : JU/SJ
Sample : J2360-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NAA-WS-003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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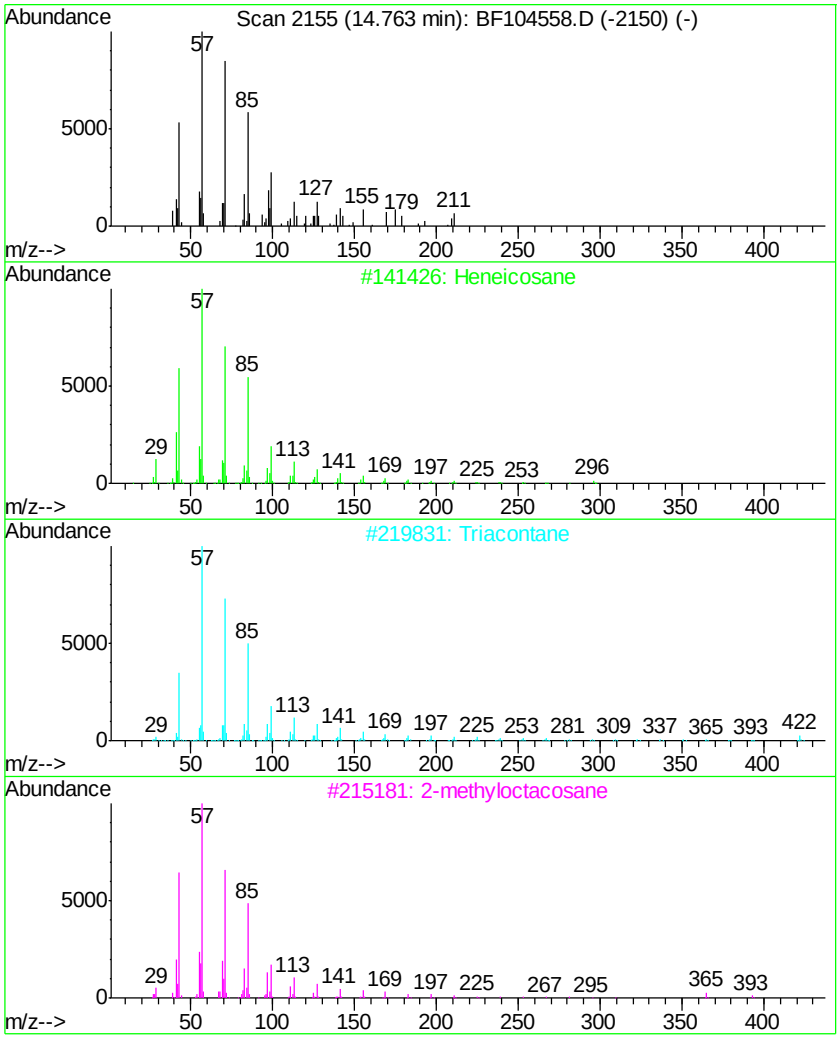
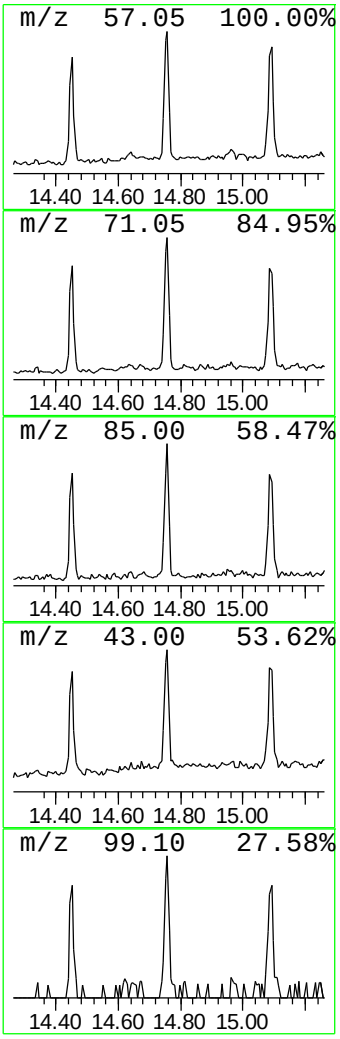
Peak Number 9 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.76	2.53 ng	88673	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Triacontane	422	C30H62	000638-68-6	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Octacosane	394	C28H58	000630-02-4	90
5	Heptacosane	380	C27H56	000593-49-7	90





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041618\
Data File : BF104558.D
Acq On : 17 Apr 2018 2:38
Operator : JU/SJ
Sample : J2360-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NAA-WS-003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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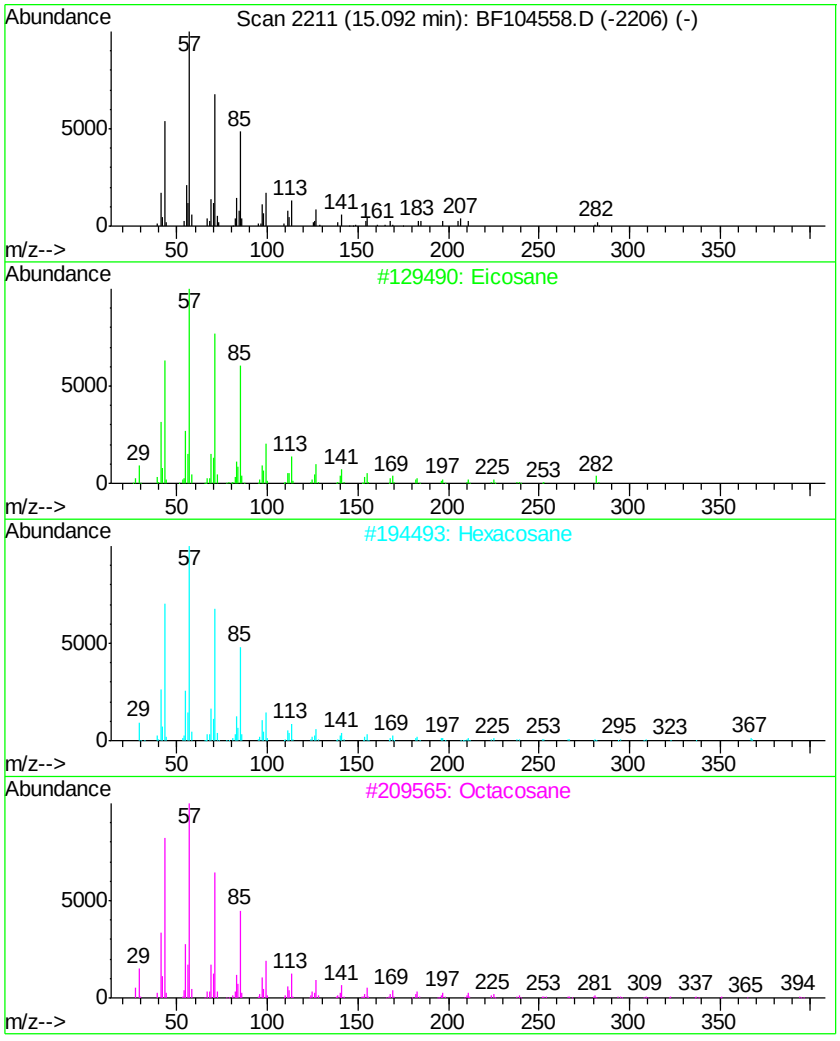
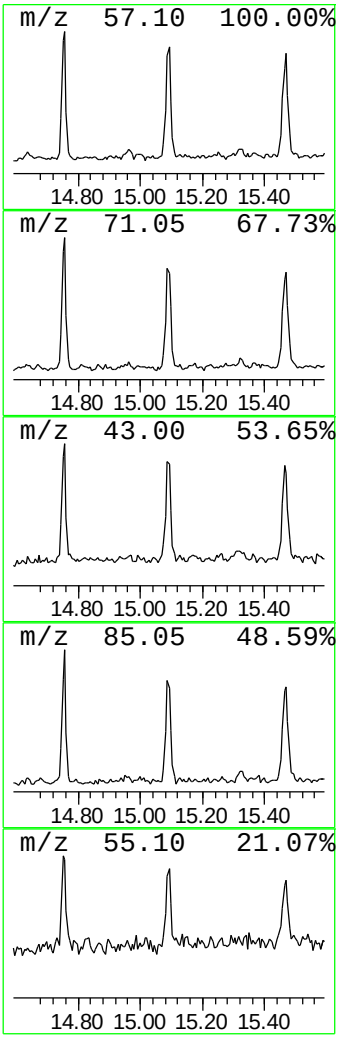
Peak Number 10 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	2.40 ng	83913	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Hexacosane	366	C26H54	000630-01-3	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041618\
Data File : BF104558.D
Acq On : 17 Apr 2018 2:38
Operator : JU/SJ
Sample : J2360-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NAA-WS-003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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
2-Pentanone, 4-hy...	5.02	3.4	ng	154022	1	6.81	902064	20.0
Ethanol, 2-(2-met...	6.06	2.0	ng	90985	1	6.81	902064	20.0
unknown6.58	6.58	65.7	ng	2963780	1	6.81	902064	20.0
Heptacosane	10.75	2.6	ng	118394	4	11.34	892668	20.0
Hexadecanoic acid...	12.75	8.2	ng	326961	5	13.99	799255	20.0
Octadecanoic acid...	13.45	5.9	ng	236934	5	13.99	799255	20.0
Octacosyl trifluo...	13.82	3.9	ng	156576	5	13.99	799255	20.0
Heneicosane	14.76	2.5	ng	88673	6	15.45	699622	20.0
Eicosane	15.09	2.4	ng	83913	6	15.45	699622	20.0