LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102253.D
Acq On : 20 Jan 2018 9:34
Operator : SJ/JU
Sample : J1114-15
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-28-2.0-2.5

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-BF010918.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	4.934	480	484	494	rVB	205351	355025	7.70%	0.834%
2	5.340	547	553	556	rBV	4027462	4442683	96.30%	10.440%
3	6.369	721	728	731	rBV	3583252	4561398	98.88%	10.719%
4	6.492	744	749	752	rBV	4261722	4501061	97.57%	10.578%
5	6.716	784	787	791	rBV	1074614	860704	18.66%	2.023%
6	6.875	809	814	817	rBV	3735376	3439559	74.56%	8.083%
7	7.287	878	884	887	rBV	2668502	2943044	63.80%	6.916%
8	7.998	1001	1005	1009	rBV	1346823	1142194	24.76%	2.684%
9	9.081	1183	1189	1192	rBV	4445544	4613175	100.00%	10.841%
10	9.469	1251	1255	1258	rBV	425371	349356	7.57%	0.821%
11	9.686	1287	1292	1296	rBV	108976	98685	2.14%	0.232%
12	9.751	1299	1303	1307	rVB	1404537	1213380	26.30%	2.851%
13	9.963	1333	1339	1343	rBV	107967	135288	2.93%	0.318%
14	10.186	1374	1377	1380	rVB2	119471	119112	2.58%	0.280%
15	10.398	1409	1413	1416	rBV2	38216	52691	1.14%	0.124%
16	10.545	1431	1438	1441	rBV	2738157	2884658	62.53%	6.779%
17	10.657	1454	1457	1461	rBV	104810	98617	2.14%	0.232%
18	10.904	1493	1499	1503	rBV5	47012	60520	1.31%	0.142%
19	11.233	1551	1555	1559	rBV	1308738	1221964	26.49%	2.872%
20	11.774	1641	1647	1650	rBV	176280	190592	4.13%	0.448%
21	12.645	1791	1795	1798	rBV2	137880	130922	2.84%	0.308%
22	12.721	1805	1808	1811	rVB	90537	78922	1.71%	0.185%
23	12.827	1821	1826	1829	rBV	3887070	4275665	92.68%	10.048%
24	13.304	1902	1907	1911	rVB	78223	88894	1.93%	0.209%
25	13.345	1911	1914	1917	rBV	82517	80133	1.74%	0.188%
26	13.374	1917	1919	1924	rVB2	53801	69087	1.50%	0.162%
27	13.716	1973	1977	1980	rBV	736532	750853	16.28%	1.765%
28	13.745	1980	1982	1993	rVB	158148	163435	3.54%	0.384%
29	13.868	1998	2003	2007	rBV	1220925	1181360	25.61%	2.776%
30	14.039	2028	2032	2039	rBV	91936	107755	2.34%	0.253%
31	14.345	2081	2084	2091	rBV	197194	227466	4.93%	0.535%
32	14.639	2128	2134	2142	rBV2	104909	169718	3.68%	0.399%
33	14.957	2185	2188	2191	rBV	109419	125424	2.72%	0.295%
34	15.292	2240	2245	2248	rBV	762098	939797	20.37%	2.209%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102253.D
Acq On : 20 Jan 2018 9:34
Operator : SJ/JU
Sample : J1114-15
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-28-2.0-2.5

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-BF010918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.727	2314	2319	2323	rBV	118275	163926	3.55%	0.385%
36	15.774	2323	2327	2334	rVB2	74420	116414	2.52%	0.274%
37	15.868	2340	2343	2349	rVB7	47886	82756	1.79%	0.194%
38	16.198	2393	2399	2405	rBV2	97996	189411	4.11%	0.445%
39	16.756	2488	2494	2499	rVB2	56886	110962	2.41%	0.261%
40	17.204	2565	2570	2578	rVB8	37436	77592	1.68%	0.182%
41	17.404	2599	2604	2612	rVB3	38729	86839	1.88%	0.204%
42	18.180	2730	2736	2743	rBV8	20982	51983	1.13%	0.122%

Sum of corrected areas: 42553020

LSC Report - Integrated Chromatogram

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Operator : SJ/JU
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Misc :
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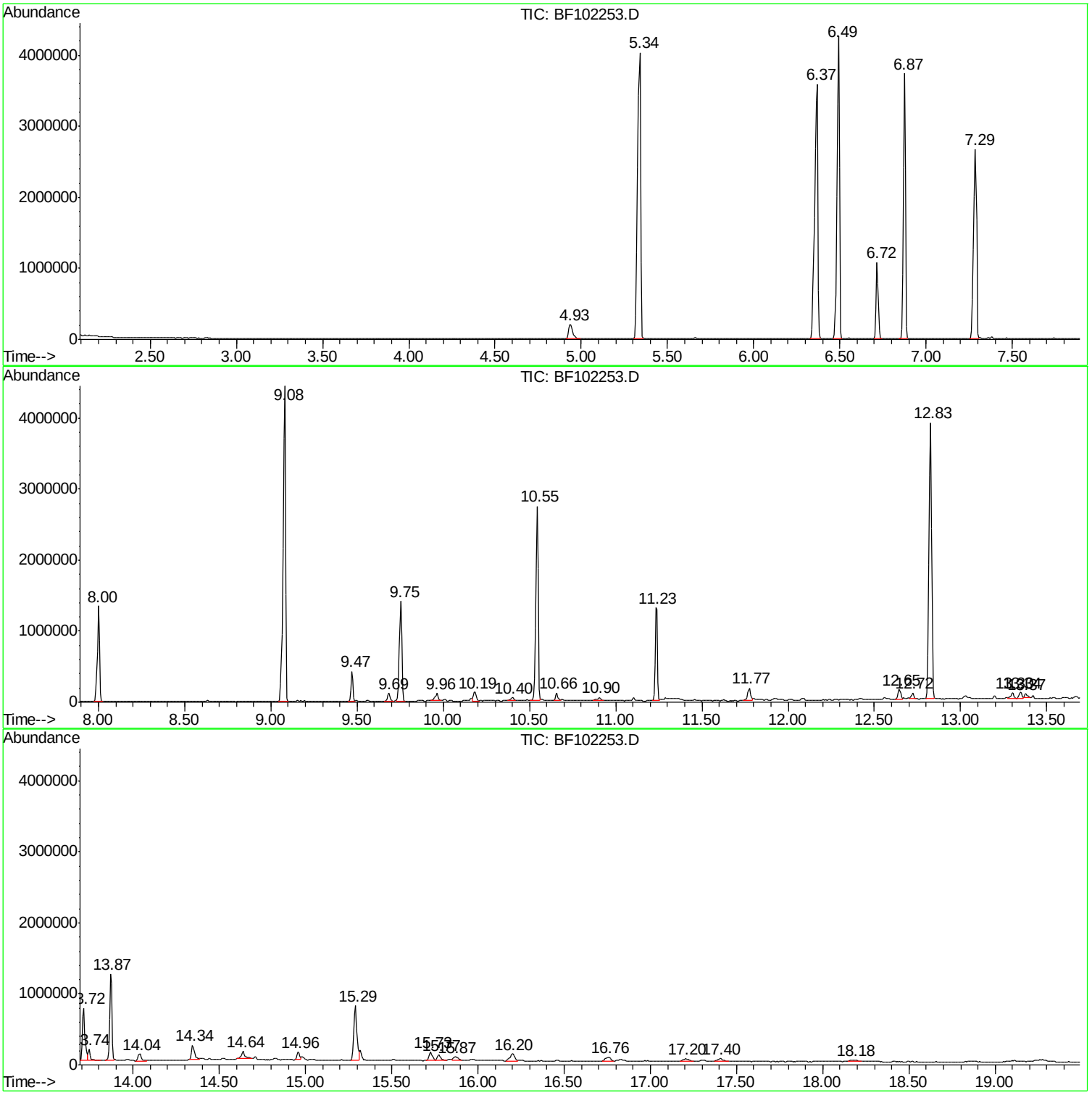
Instrument : BNA_F
ClientSampleId : SB-28-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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\BF012018\
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Operator : SJ/JU
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Misc :
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Instrument : BNA_F
ClientSampleId : SB-28-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

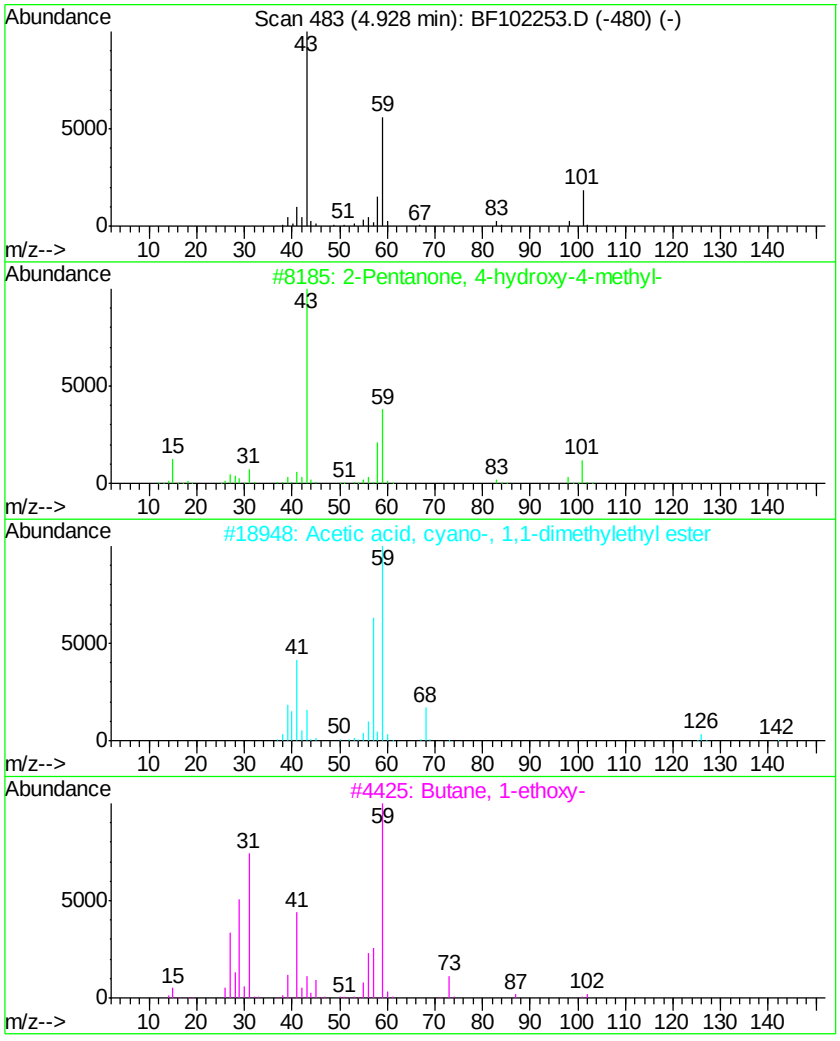
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

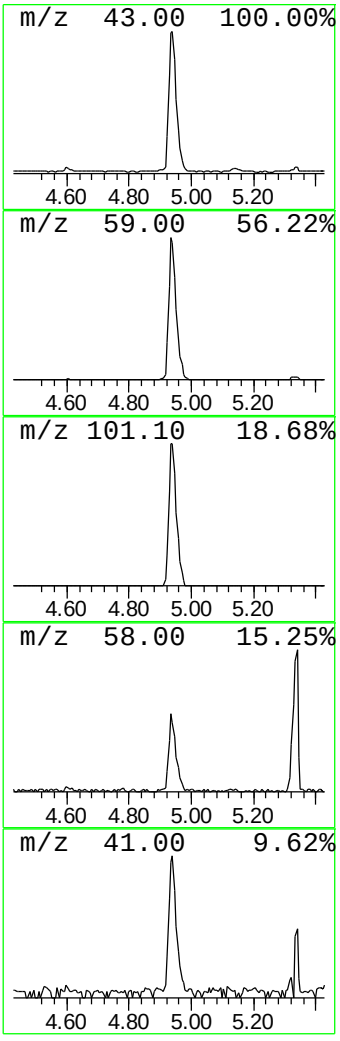
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	8.25 ng	355025	1,4-Dichlorobenzene-d4	6.72

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Instrument : BNA_F
ClientSampleId : SB-28-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

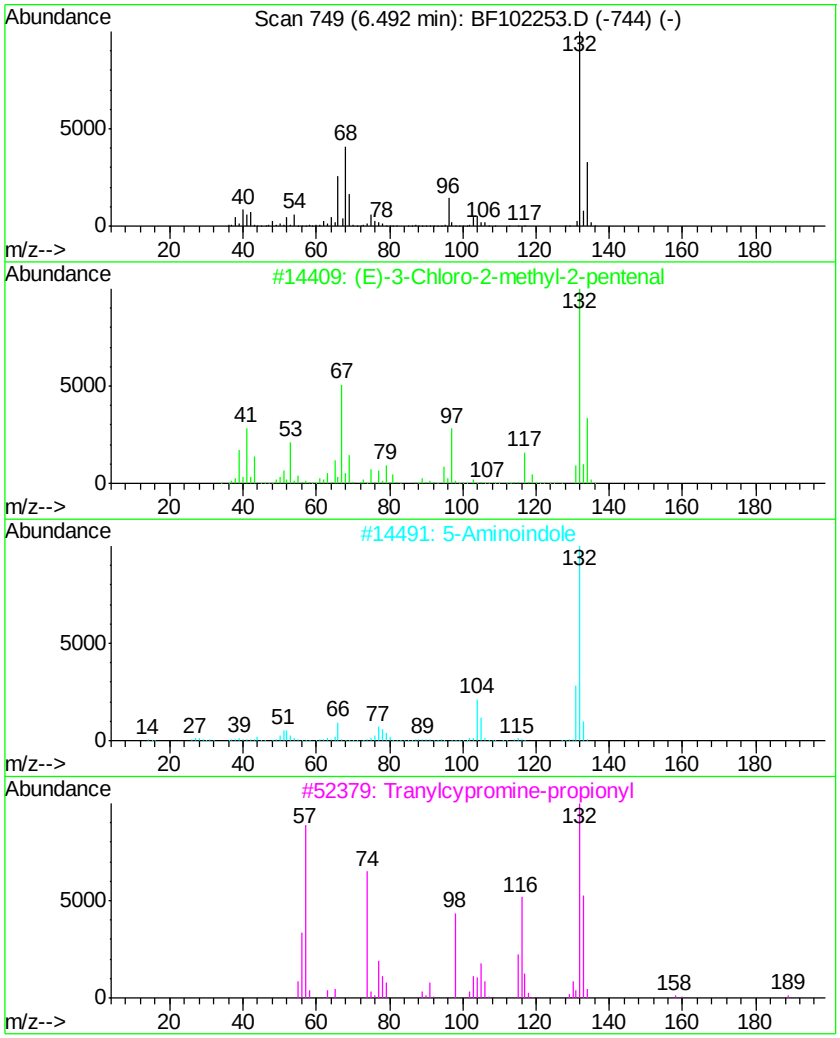
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

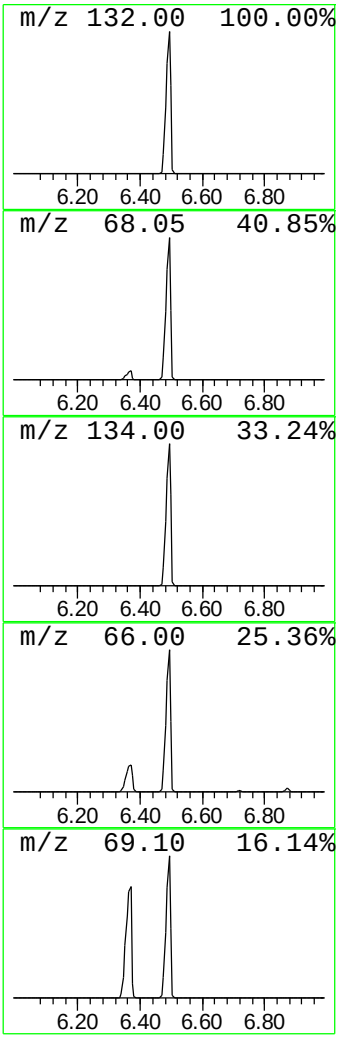
****

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	104.59 ng	4501060	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Sample : J1114-15
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-28-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

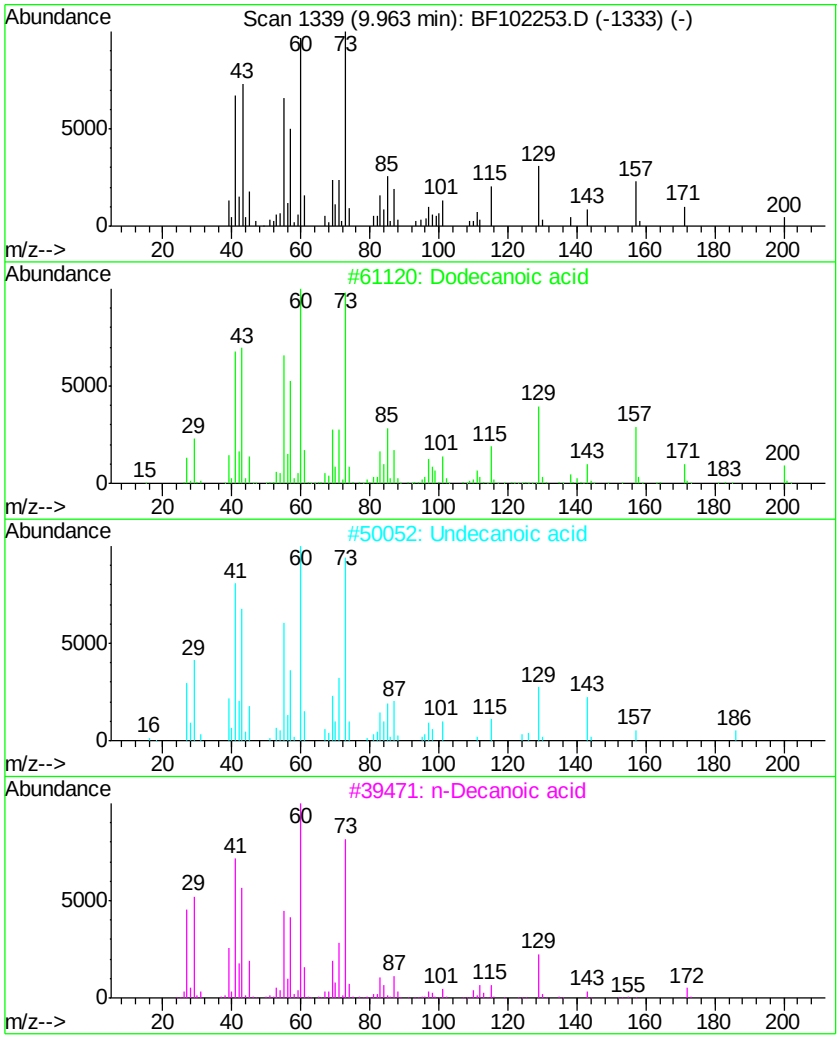
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

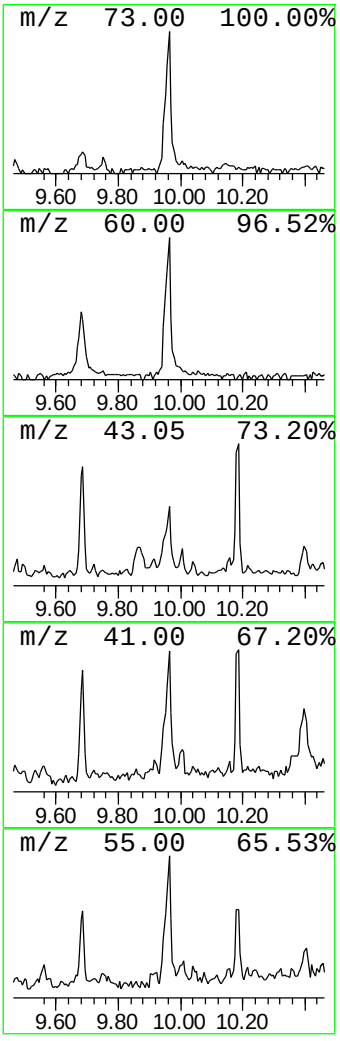
****

Peak Number 4 Dodecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.96	2.23 ng	135288	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	97
2	Undecanoic acid	186	C11H22O2	000112-37-8	59
3	n-Decanoic acid	172	C10H20O2	000334-48-5	50
4	Octanoic acid	144	C8H16O2	000124-07-2	47
5	Hexanoic acid	116	C6H12O2	000142-62-1	38





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
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Operator : SJ/JU
Sample : J1114-15
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-28-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
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TIC Library : C:\DATABASE\NIST11.L
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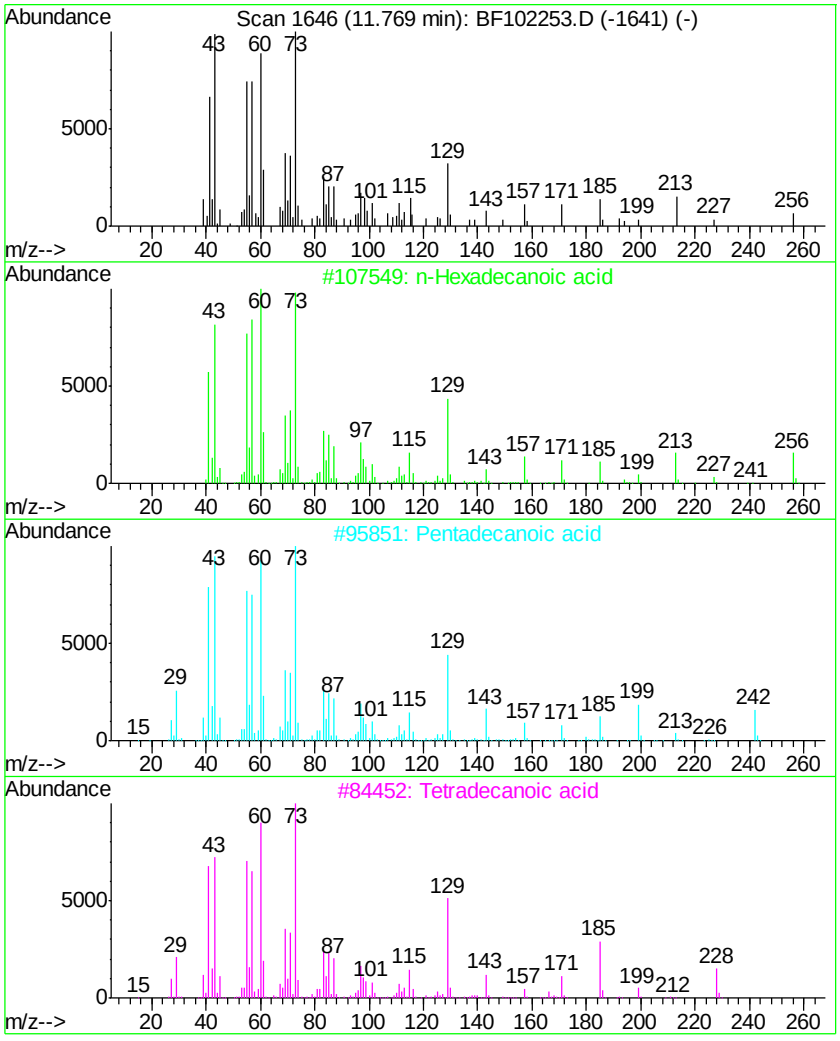
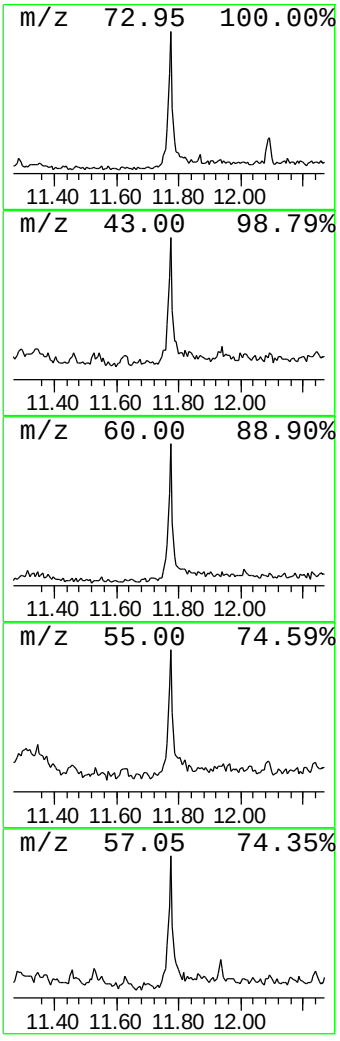
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	3.12 ng	190592	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20





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Sample : J1114-15
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-28-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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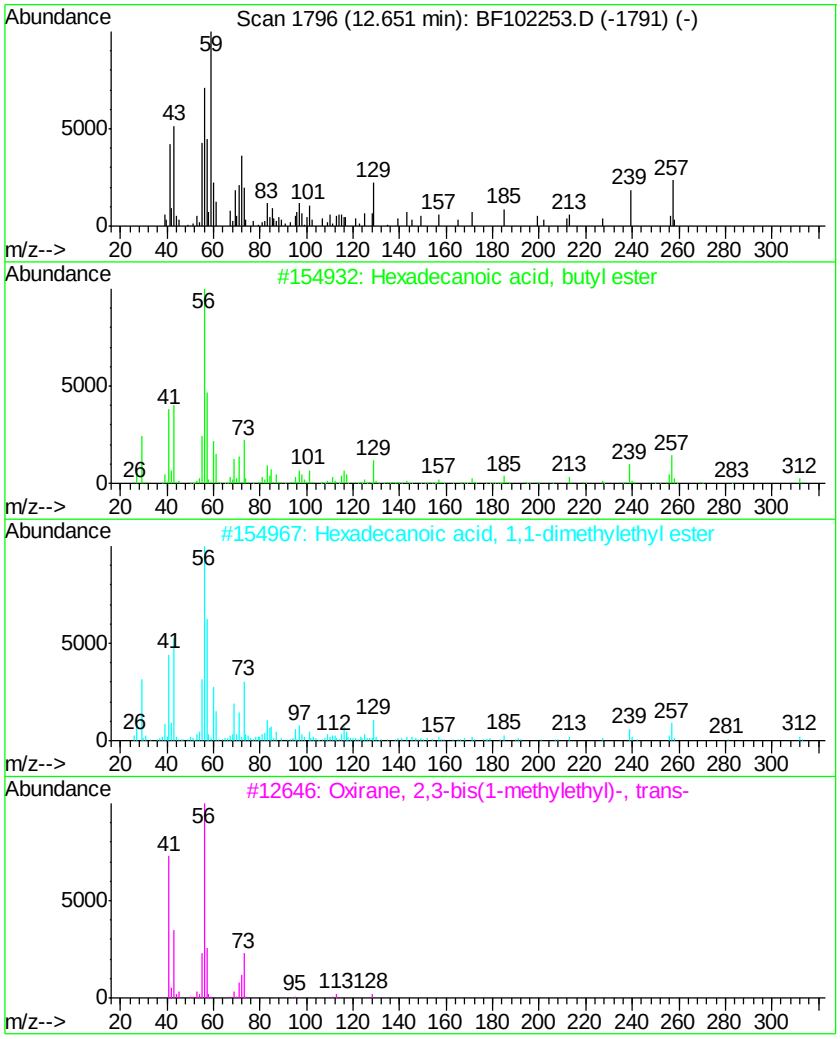
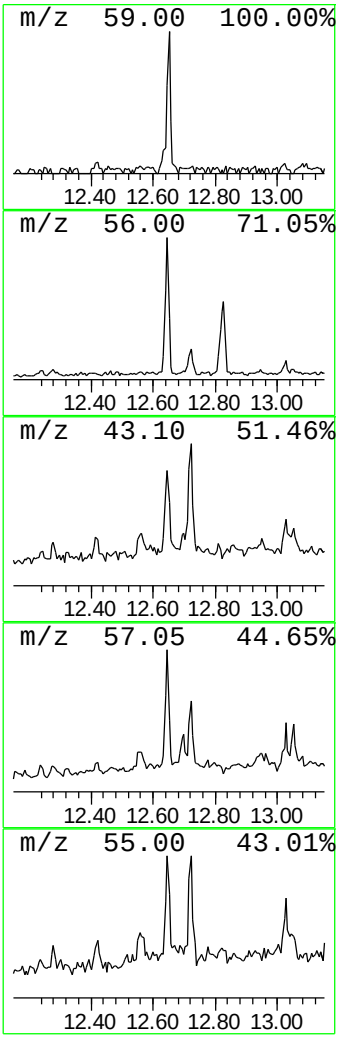
Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	2.22 ng	130922	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	64
3	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	35
4	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	30
5	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	27





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Instrument : BNA_F
ClientSampleId : SB-28-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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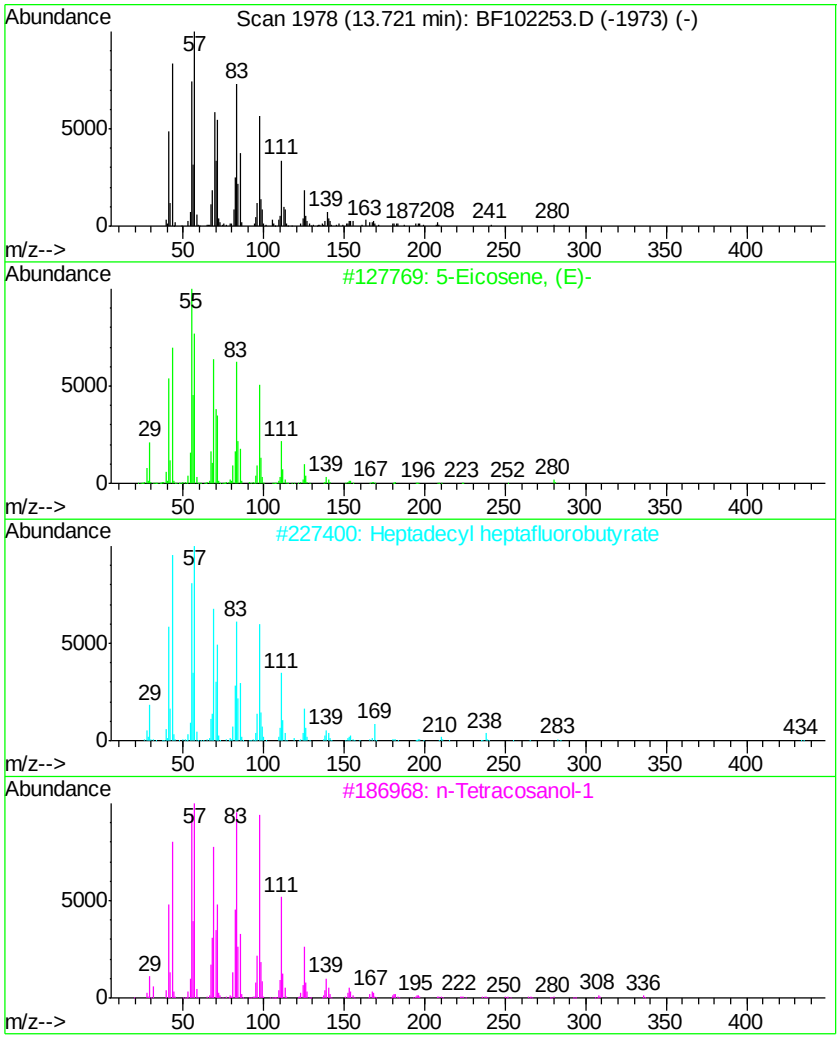
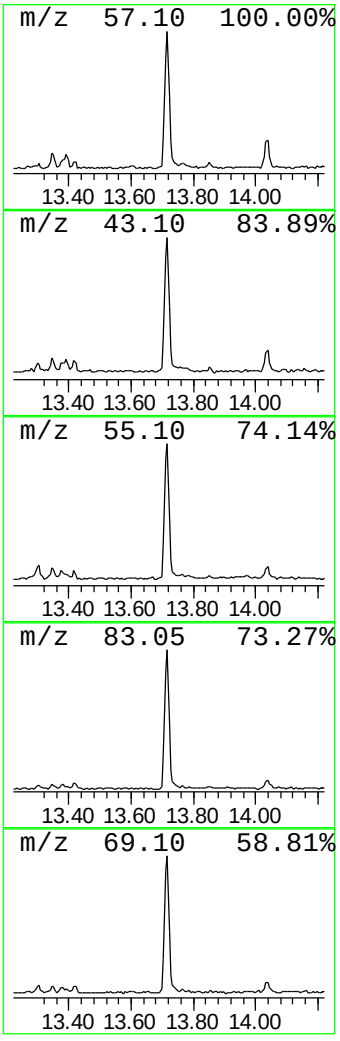
Peak Number 7 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	12.71 ng	750853	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Behenic alcohol	326	C22H46O	000661-19-8	93





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TIC Library : C:\DATABASE\NIST11.L
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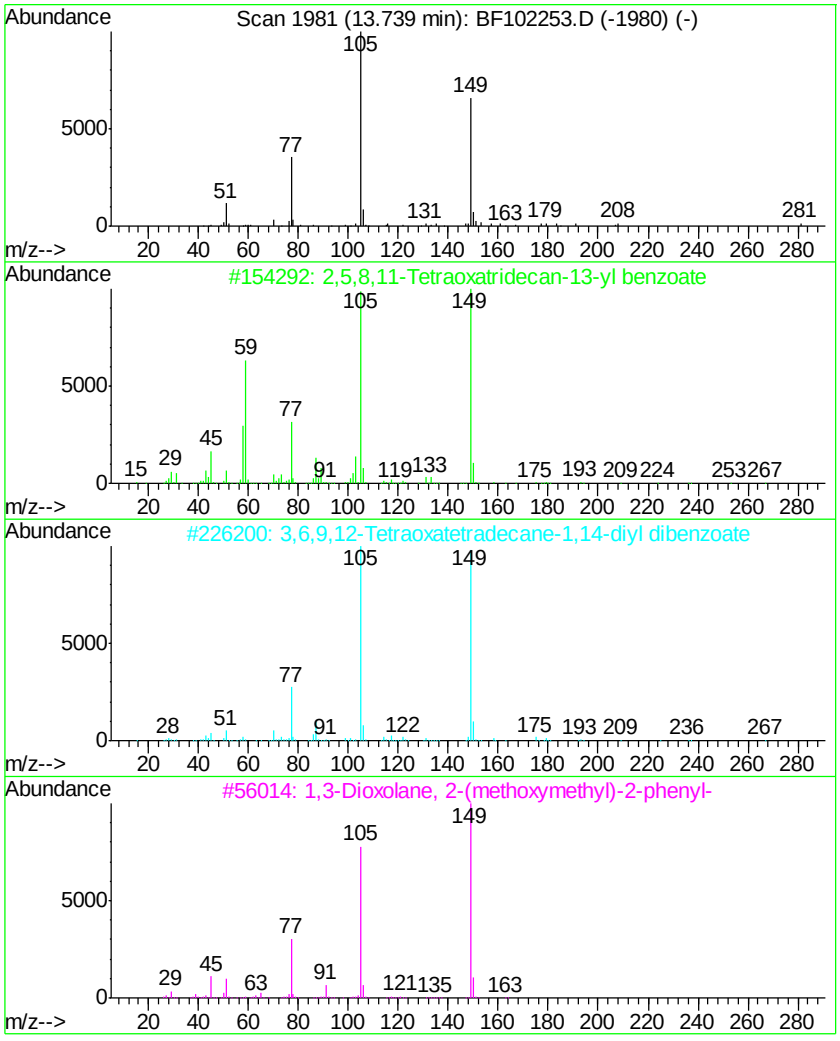
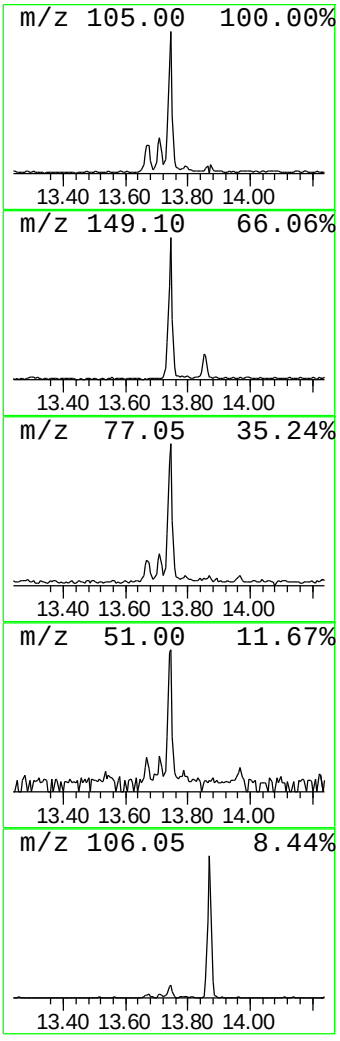
Peak Number 8 2,5,8,11-Tetraoxatridecan-1... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	2.77 ng	163435	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5,8,11-Tetraoxatridecan-13-yl ...	312	C16H24O6	1000366-96-7	78
2	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	78
3	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	78
4	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	78
5	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	78





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Instrument : BNA_F
ClientSampleId : SB-28-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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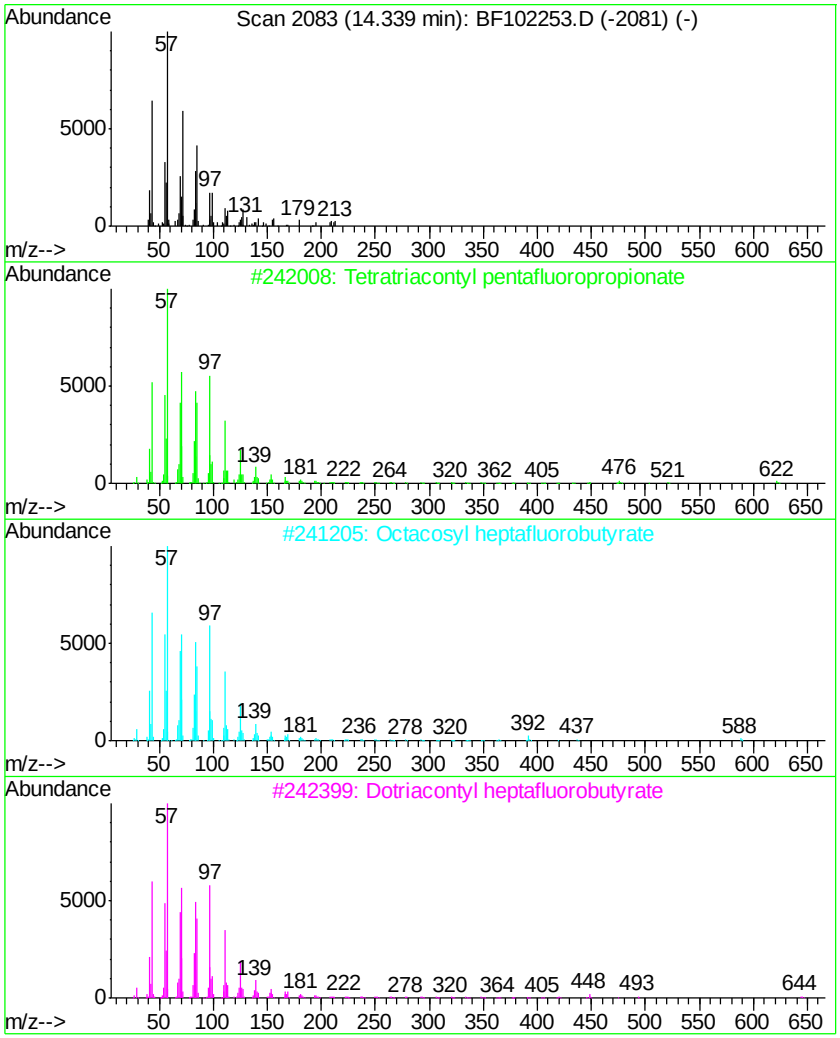
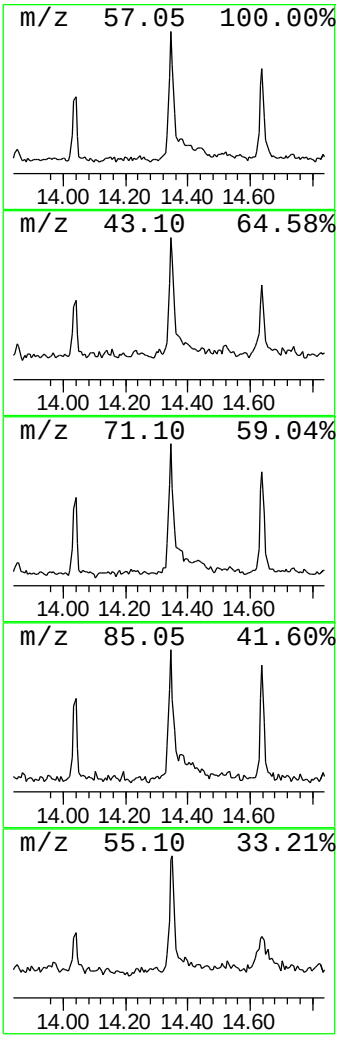
Peak Number 9 Tetratriacontyl pentafluoro... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	3.85 ng	227466	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	91
2	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	87
3	Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	87
4	Triacontyl trifluoroacetate	534	C32H61F3O2	1000351-75-7	87
5	Tetratriacontyl trifluoroacetate	591	C36H69F3O2	1000351-75-3	87





Library Search Compound Report

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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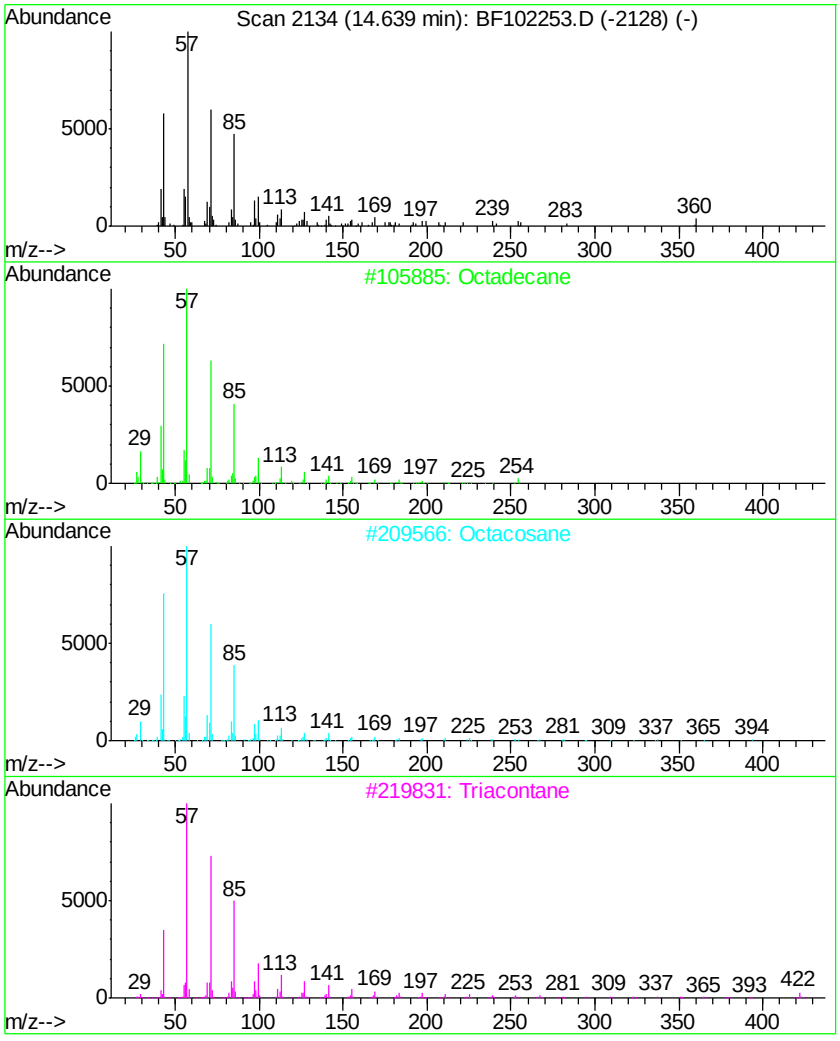
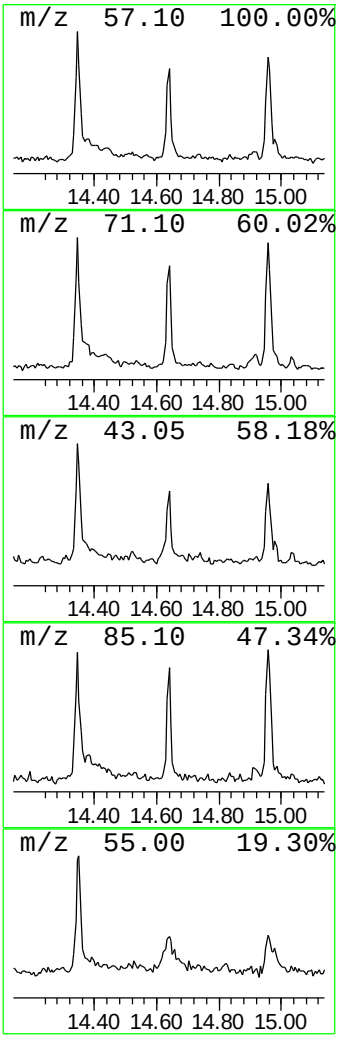
Peak Number 10 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	3.61 ng	169718	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	96
2	Octacosane	394	C28H58	000630-02-4	90
3	Triacontane	422	C30H62	000638-68-6	87
4	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	87
5	Tetratetracontane	619	C44H90	007098-22-8	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102253.D
Acq On : 20 Jan 2018 9:34
Operator : SJ/JU
Sample : J1114-15
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-28-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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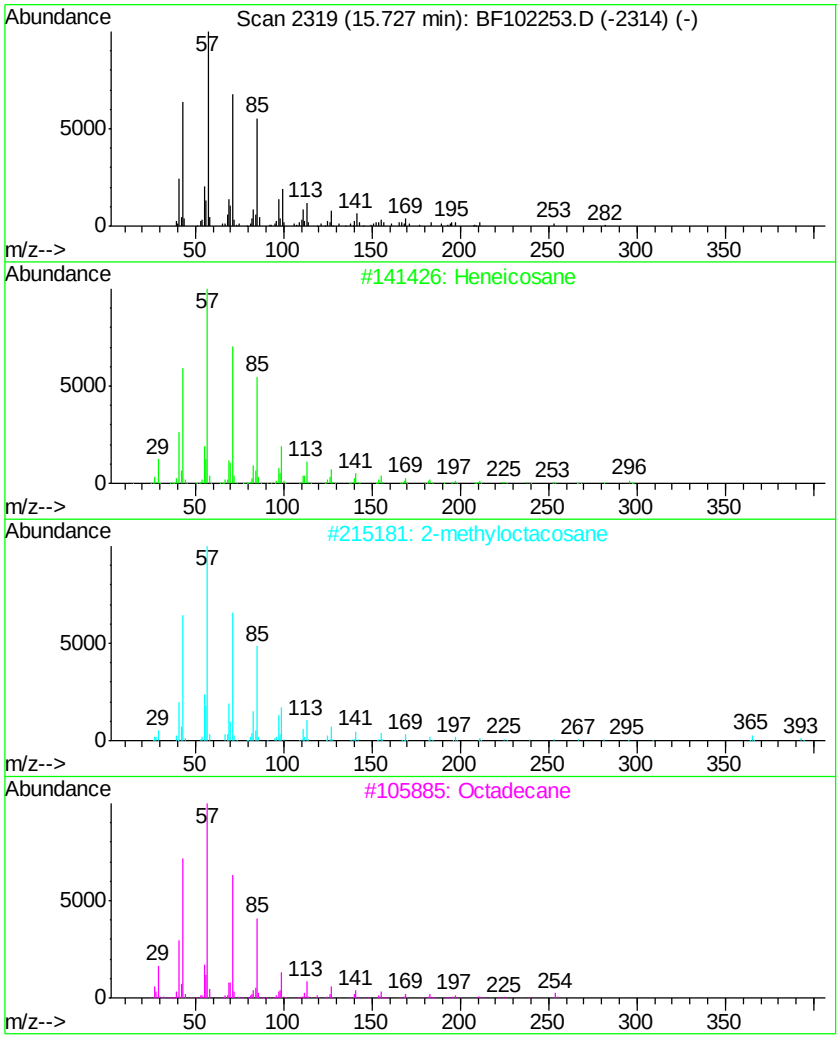
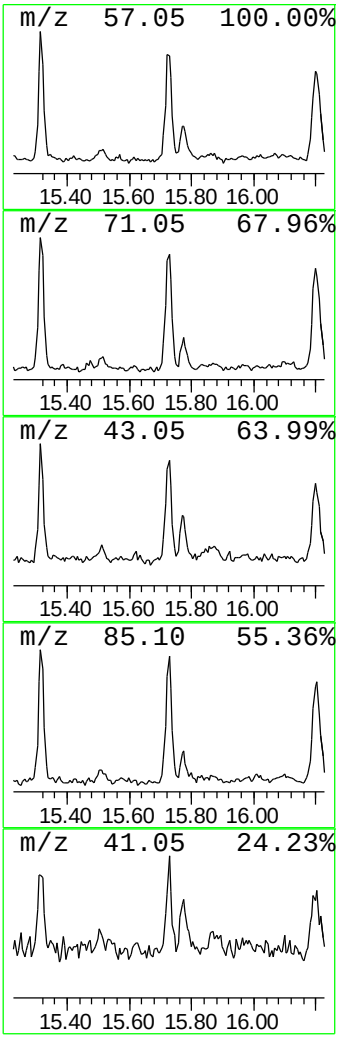
Peak Number 12 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.73	3.49 ng	163926	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	2-methyloctacosane	408	C29H60	1000376-72-8	90
3	Octadecane	254	C18H38	000593-45-3	87
4	Tetratetracontane	619	C44H90	007098-22-8	87
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86





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Data File : BF102253.D
Acq On : 20 Jan 2018 9:34
Operator : SJ/JU
Sample : J1114-15
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-28-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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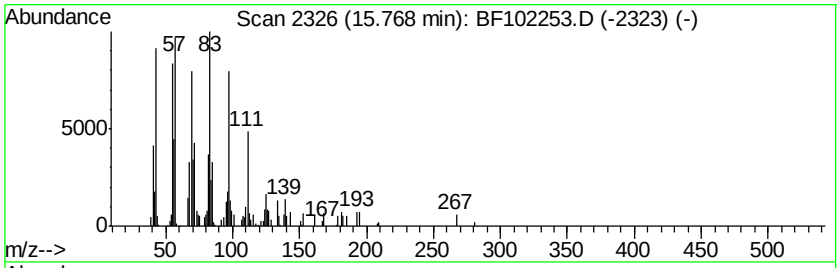
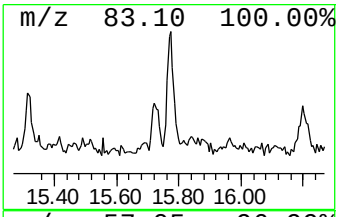
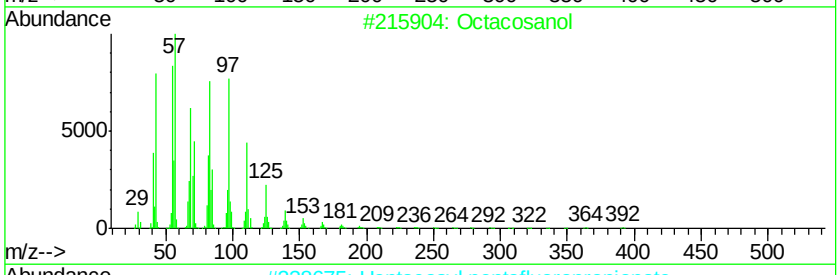
Peak Number 13 Octacosanol Concentration Rank 12

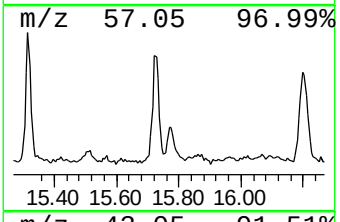
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	2.48 ng	116414	Perylene-d12	15.29

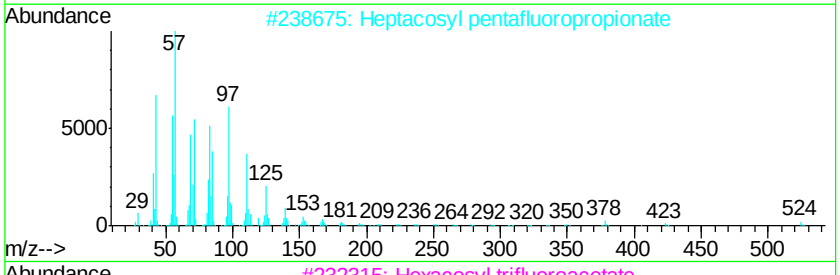
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	93
2	Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	87
3	Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	87
4	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	87
5	Behenic alcohol	326	C22H46O	000661-19-8	87

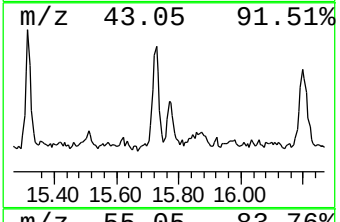


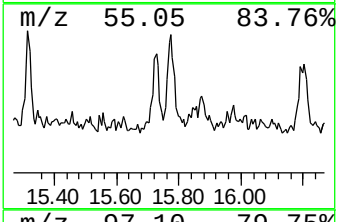


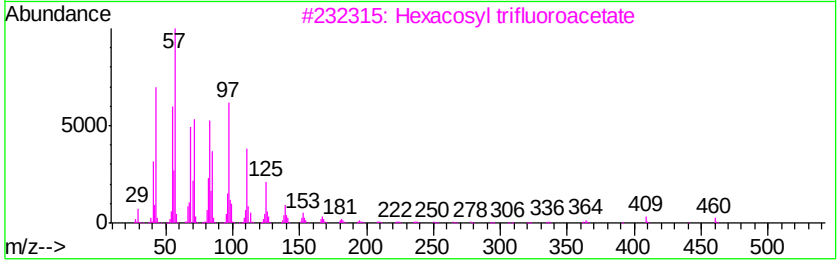


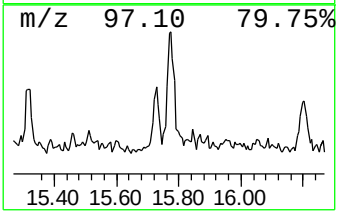












Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102253.D
Acq On : 20 Jan 2018 9:34
Operator : SJ/JU
Sample : J1114-15
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-28-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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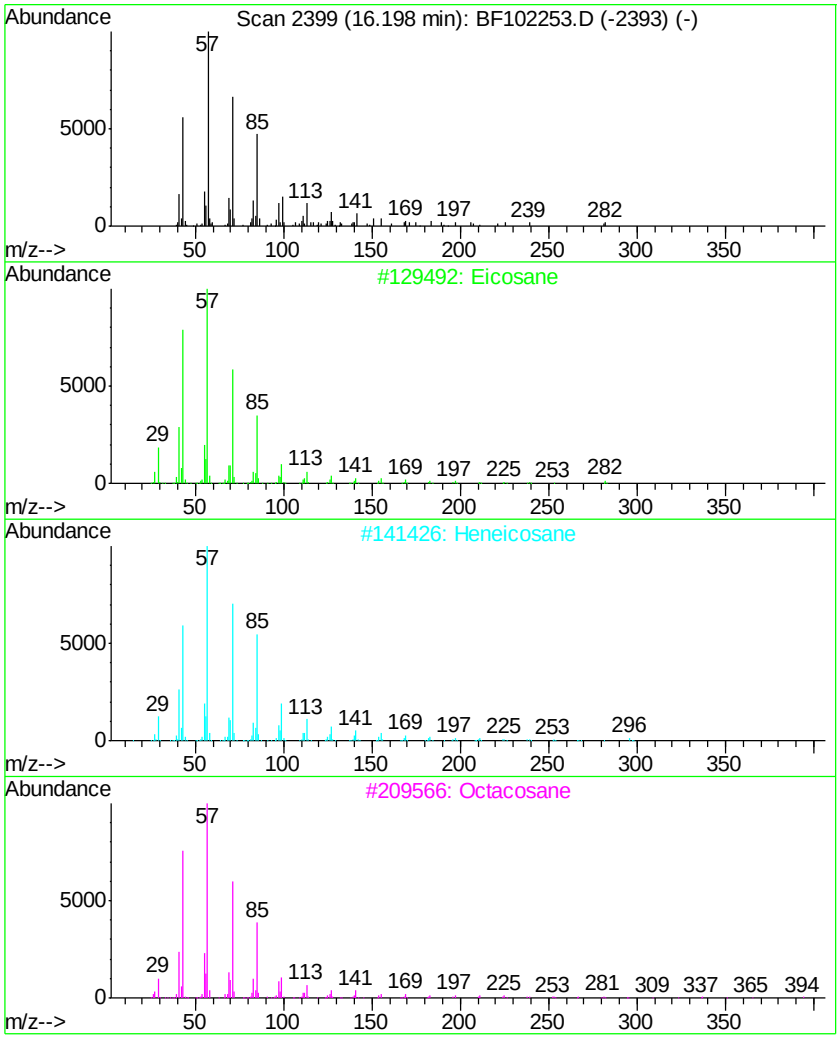
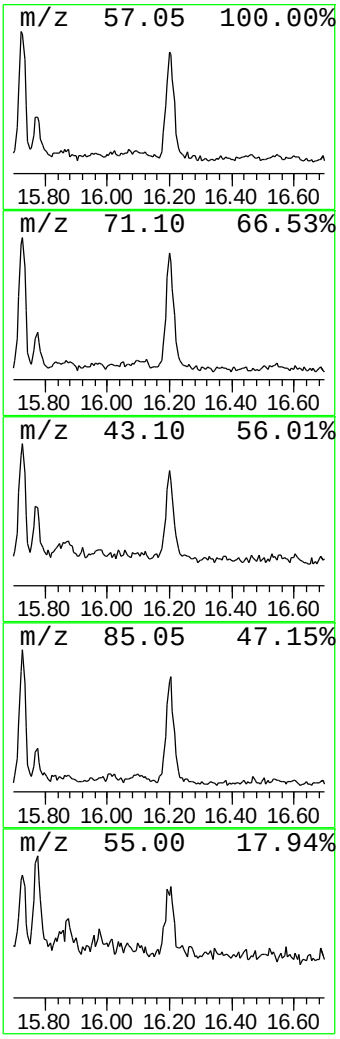
Peak Number 14 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.20	4.03 ng	189411	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Eicosane, 2-methyl-	296	C21H44	001560-84-5	90
5	Triacontane	422	C30H62	000638-68-6	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
Data File : BF102253.D
Acq On : 20 Jan 2018 9:34
Operator : SJ/JU
Sample : J1114-15
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-28-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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...	4.93	8.3	ng	355025	1	6.72	860704	20.0
unknown6.49	6.49	104.6	ng	4501060	1	6.72	860704	20.0
Dodecanoic acid	9.96	2.2	ng	135288	3	9.75	1213380	20.0
n-Hexadecanoic acid	11.77	3.1	ng	190592	4	11.23	1221960	20.0
Hexadecanoic acid...	12.65	2.2	ng	130922	5	13.87	1181360	20.0
5-Eicosene, (E)-	13.72	12.7	ng	750853	5	13.87	1181360	20.0
2,5,8,11-Tetraoxa...	13.74	2.8	ng	163435	5	13.87	1181360	20.0
Tetratriacontyl p...	14.34	3.9	ng	227466	5	13.87	1181360	20.0
Octadecane	14.64	3.6	ng	169718	6	15.29	939797	20.0
Heneicosane	15.73	3.5	ng	163926	6	15.29	939797	20.0
Octacosanol	15.77	2.5	ng	116414	6	15.29	939797	20.0
Eicosane	16.20	4.0	ng	189411	6	15.29	939797	20.0