LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042519\
Data File : BF113987.D
Acq On : 25 Apr 2019 19:36
Operator : JU/SJ
Sample : K2555-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HW-15

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-BF042219.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	2.152	6	11	18	rVB	151990	204591	4.45%	0.829%
2	5.510	578	582	598	rBV	1219791	1117714	24.30%	4.529%
3	6.516	749	753	763	rBV	797930	722876	15.72%	2.929%
4	6.663	774	778	781	rBV	2480756	2158782	46.94%	8.748%
5	6.892	814	817	821	rBV	639239	533367	11.60%	2.161%
6	7.051	840	844	848	rBV	2237131	1926257	41.88%	7.806%
7	7.451	907	912	915	rBV	1685516	1610558	35.02%	6.527%
8	8.175	1032	1035	1058	rVB	724833	686710	14.93%	2.783%
9	9.251	1214	1218	1221	rBV	3726159	3252897	70.72%	13.182%
10	9.933	1330	1334	1348	rVB	842011	855202	18.59%	3.466%
11	10.716	1463	1467	1486	rBV	2217763	2514015	54.66%	10.188%
12	11.416	1582	1586	1594	rBV	1067598	990953	21.55%	4.016%
13	11.939	1672	1675	1684	rBV2	178837	191488	4.16%	0.776%
14	12.721	1805	1808	1817	rBV	111927	143957	3.13%	0.583%
15	13.004	1851	1856	1859	rBV	4593202	4599456	100.00%	18.639%
16	14.051	2028	2034	2046	rVB	1136617	1172752	25.50%	4.752%
17	14.215	2059	2062	2070	rVB	43889	47286	1.03%	0.192%
18	14.527	2110	2115	2119	rVB2	82052	88714	1.93%	0.360%
19	14.839	2164	2168	2172	rBV	129464	124929	2.72%	0.506%
20	15.186	2223	2227	2232	rVB	148009	168344	3.66%	0.682%
21	15.539	2282	2287	2291	rBV	777786	1056898	22.98%	4.283%
22	15.574	2291	2293	2298	rVB	163943	175165	3.81%	0.710%
23	16.015	2362	2368	2376	rBV	106996	168137	3.66%	0.681%
24	16.533	2451	2456	2463	rVB2	64694	111623	2.43%	0.452%
25	17.139	2554	2559	2569	rVB4	27410	54188	1.18%	0.220%

Sum of corrected areas: 24676859

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Misc :
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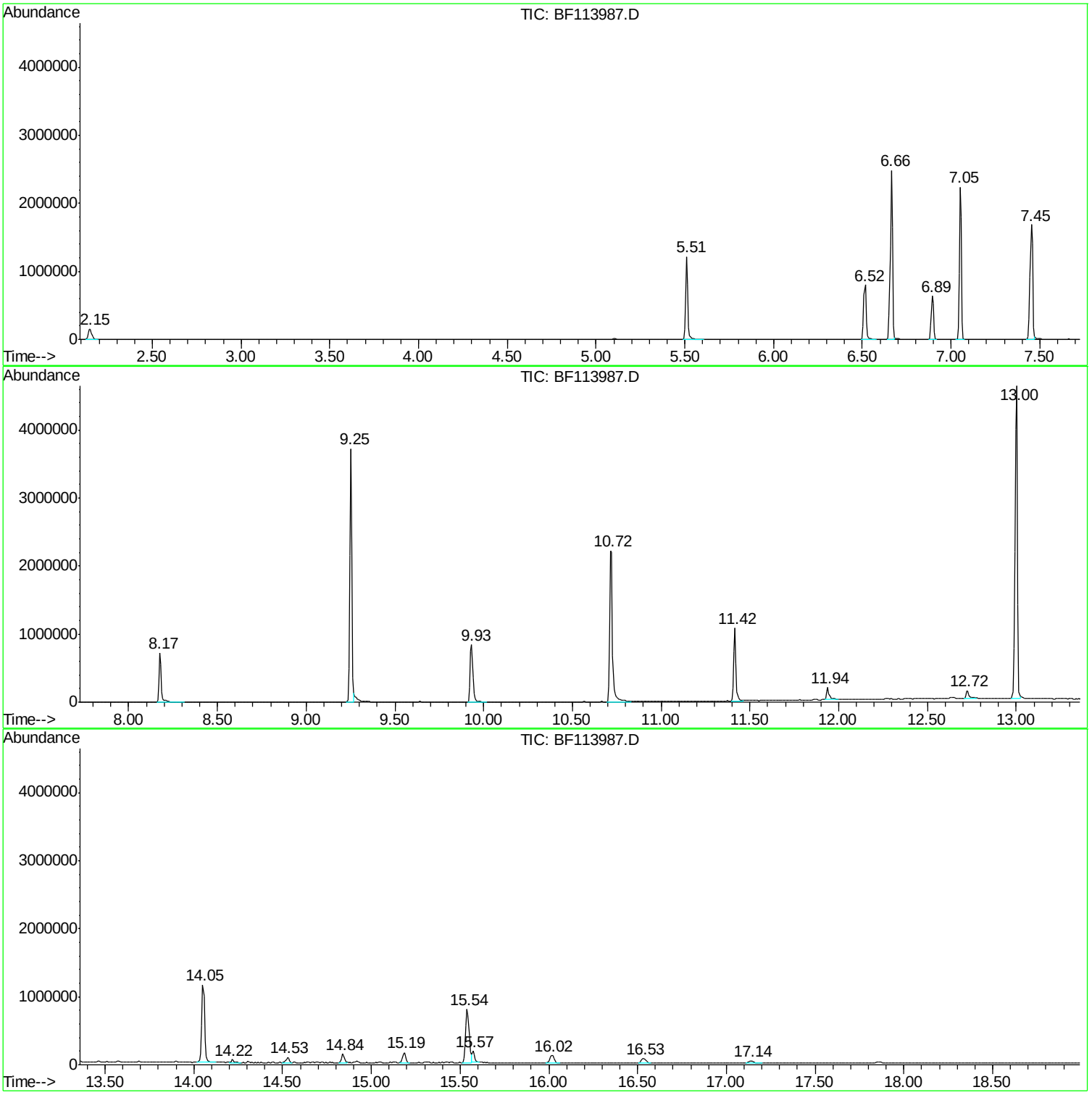
Instrument :
BNA_F
ClientSampleId :
HW-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.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 : BF113987.D
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Operator : JU/SJ
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Instrument : BNA_F
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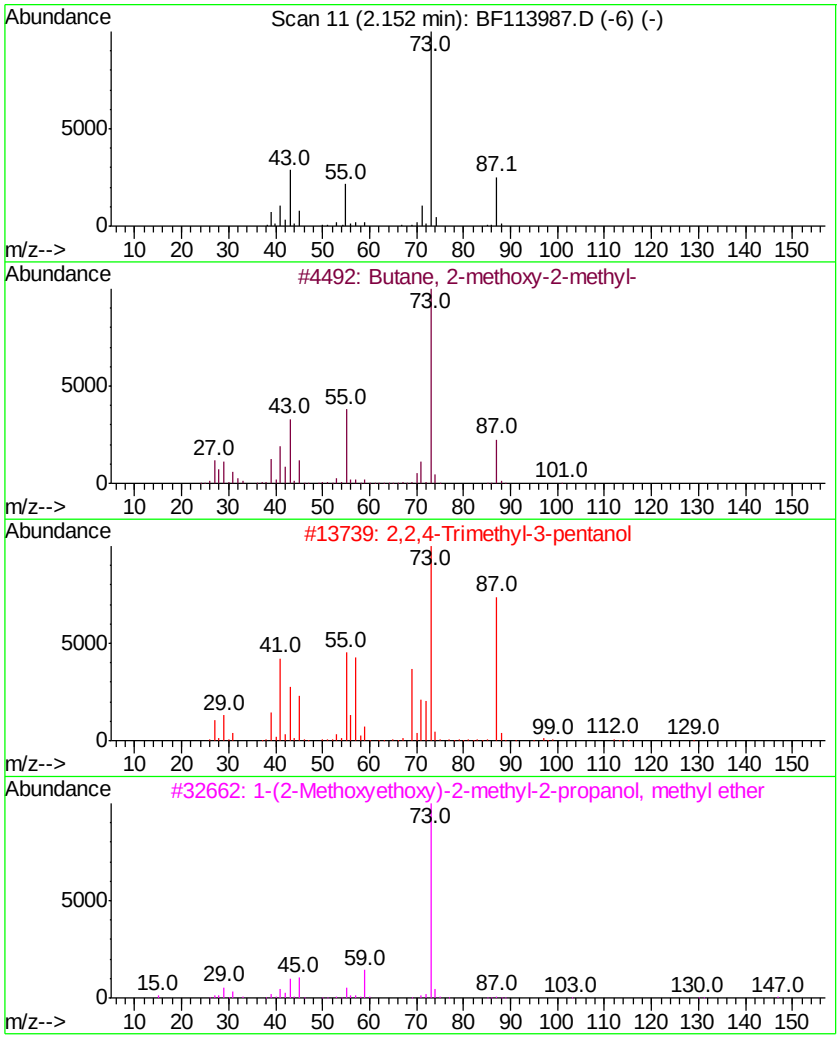
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

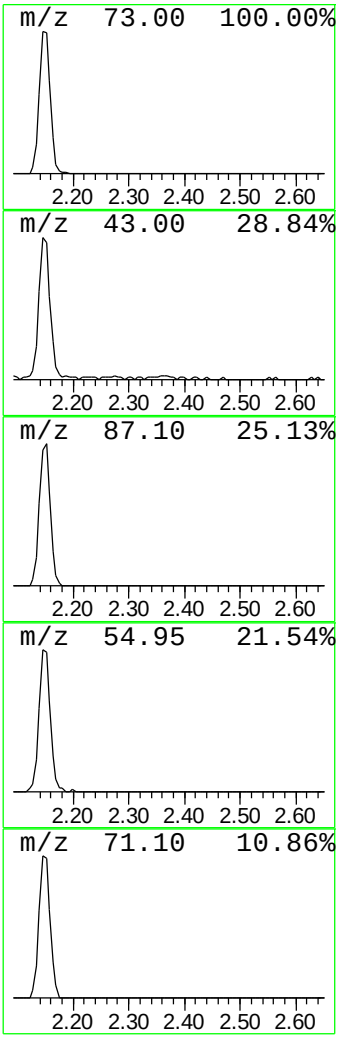
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	7.67 ng	204591	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





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Data File : BF113987.D
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Operator : JU/SJ
Sample : K2555-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HW-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

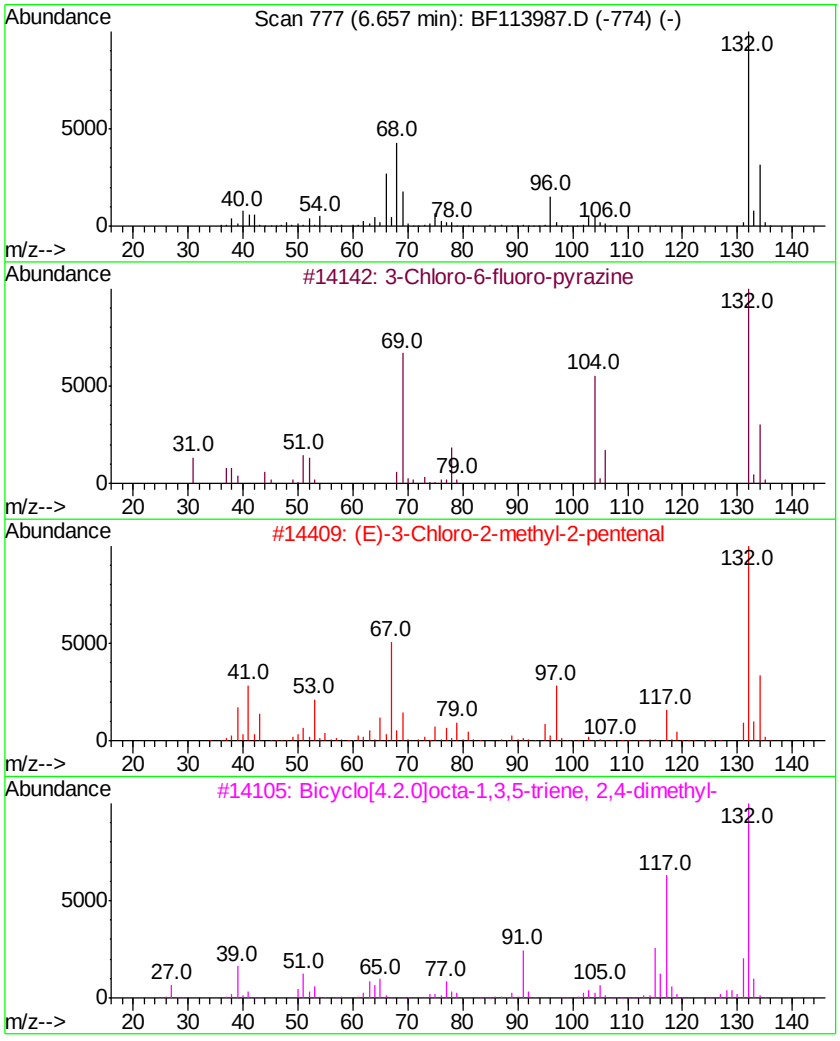
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

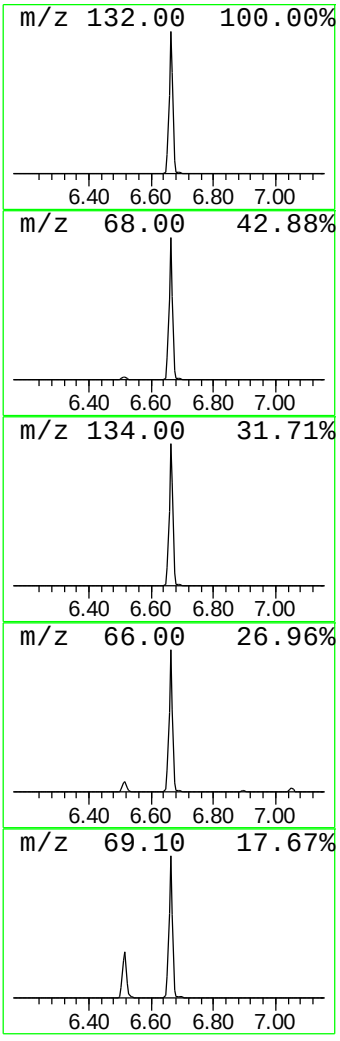
****

Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	80.95 ng	2158780	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

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Data File : BF113987.D
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Operator : JU/SJ
Sample : K2555-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HW-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

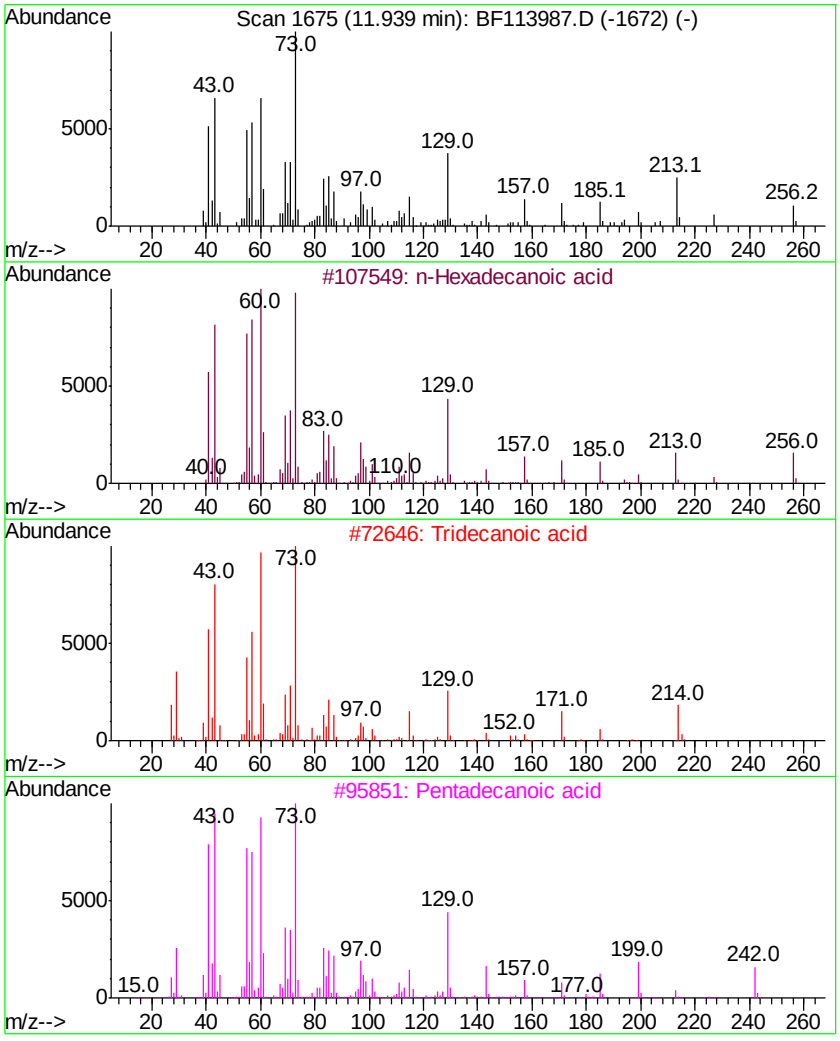
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

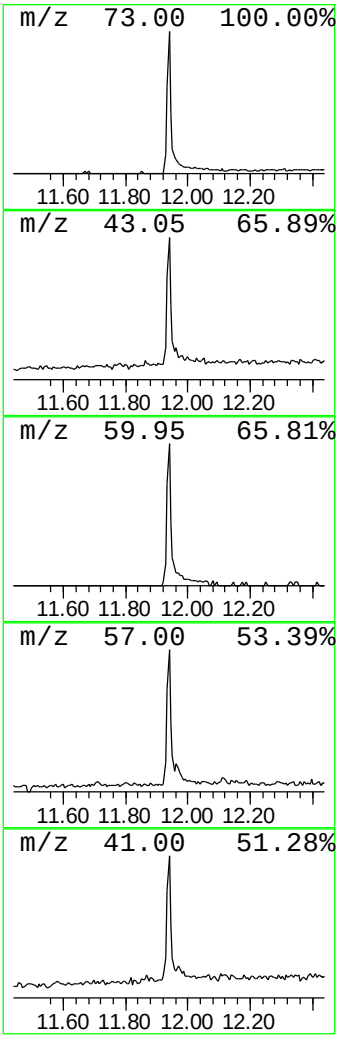
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	3.86 ng	191488	Phenanthrene-d10	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5	Dodecanoic acid	200	C12H24O2	000143-07-7	50





Library Search Compound Report

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Data File : BF113987.D
Acq On : 25 Apr 2019 19:36
Operator : JU/SJ
Sample : K2555-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HW-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

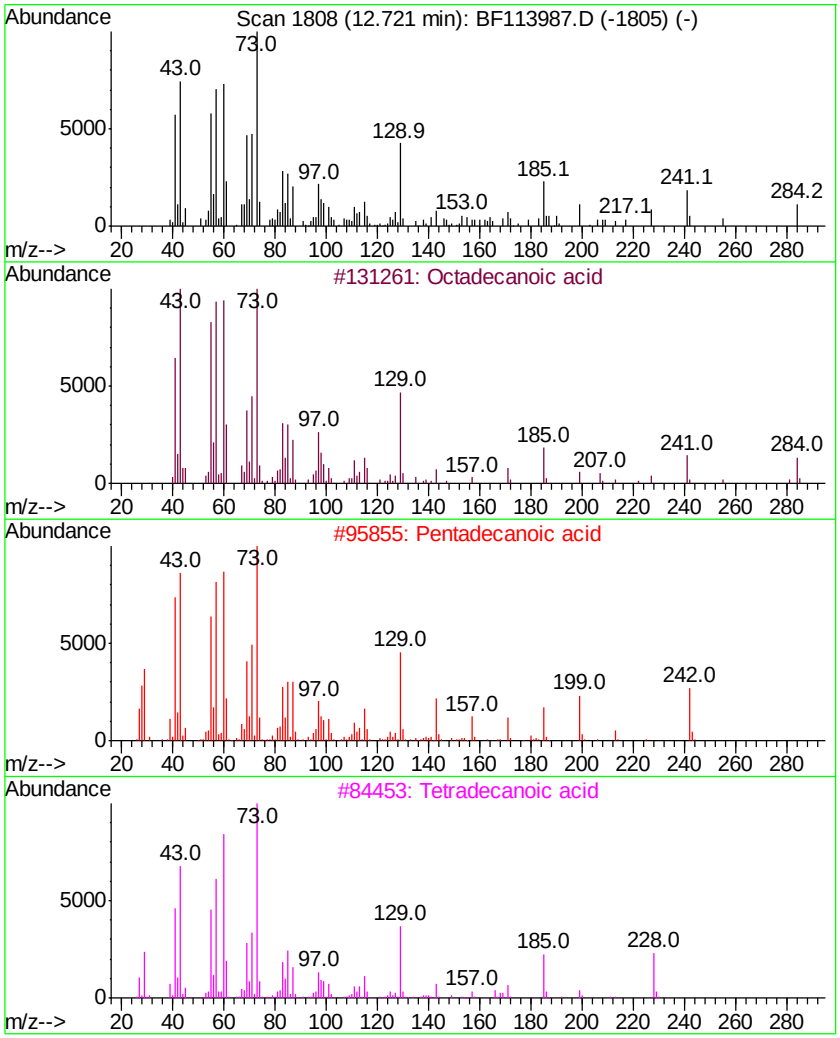
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

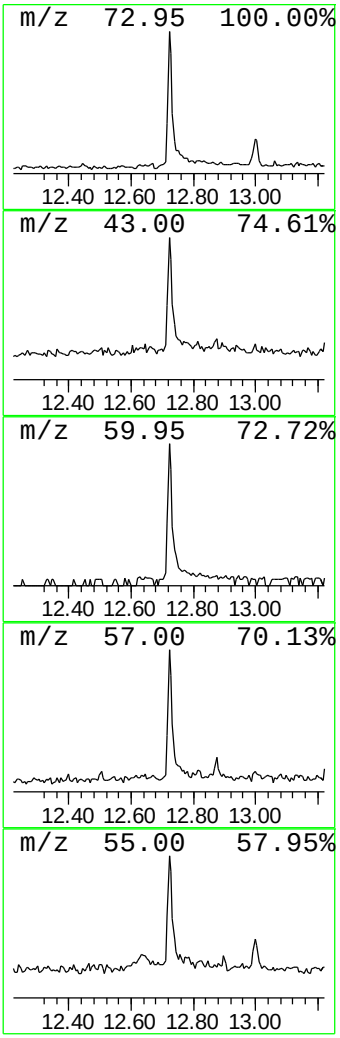
****

Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	2.91 ng	143957	Phenanthrene-d10	11.42

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	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	n-Decanoic acid	172	C10H20O2	000334-48-5	62
5	Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	35





Library Search Compound Report

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Operator : JU/SJ
Sample : K2555-06
Misc :
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Instrument : BNA_F
ClientSampleId : HW-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

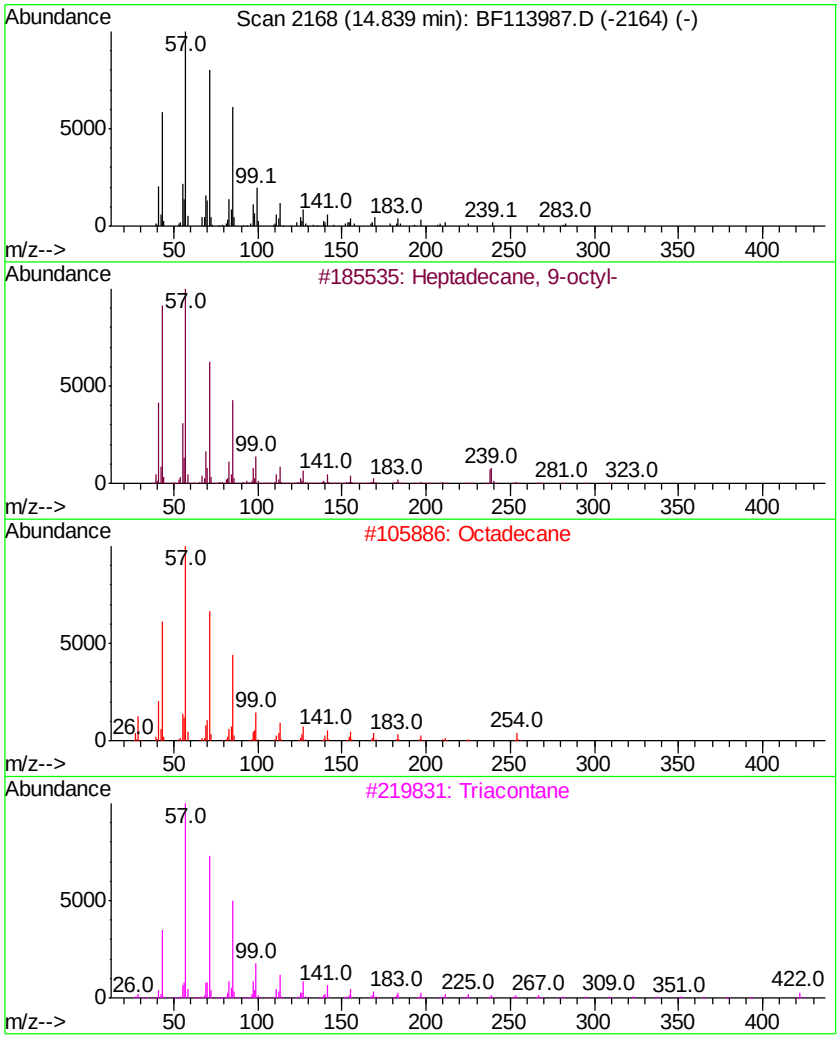
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

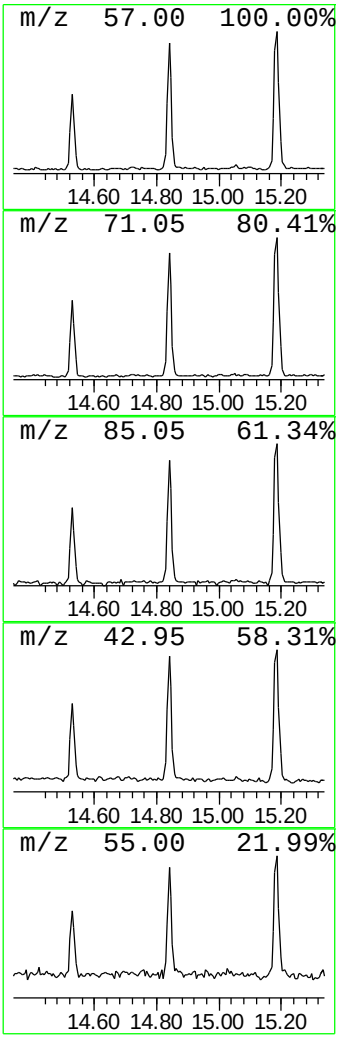
****

Peak Number 6 Heptadecane, 9-octyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	2.36 ng	124929	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Octadecane	254	C18H38	000593-45-3	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Eicosane	282	C20H42	000112-95-8	91
5	Heneicosane	296	C21H44	000629-94-7	91





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Operator : JU/SJ
Sample : K2555-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HW-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

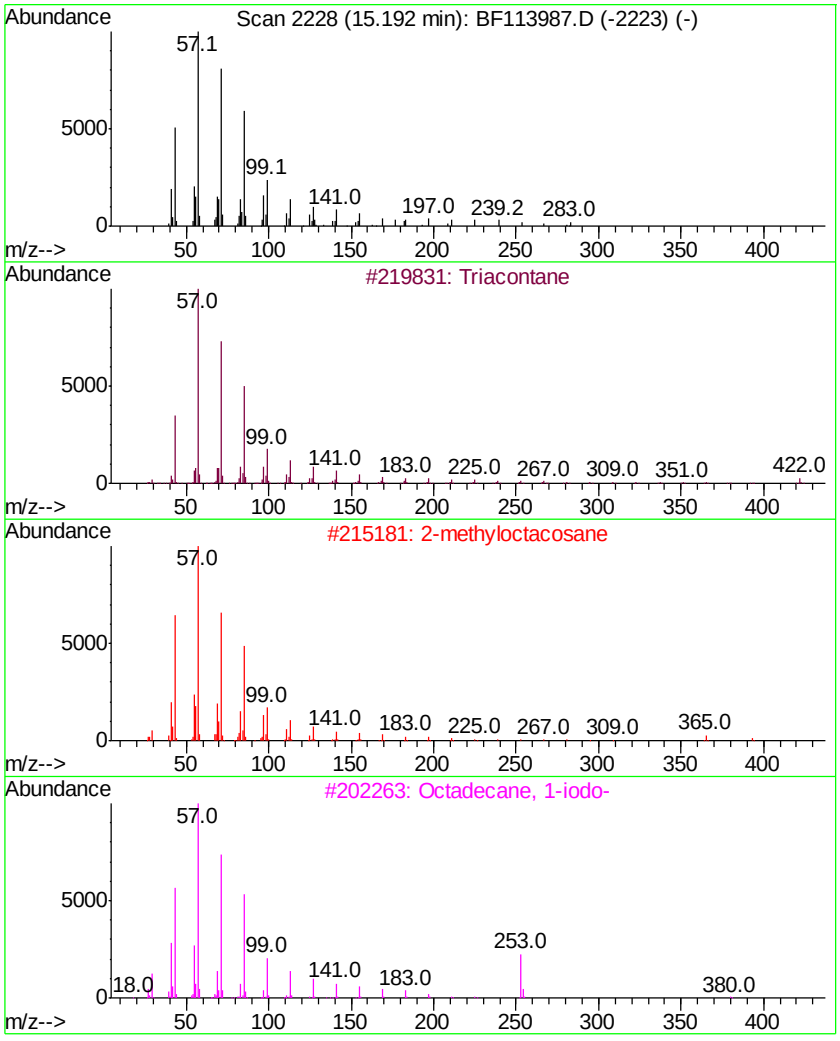
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

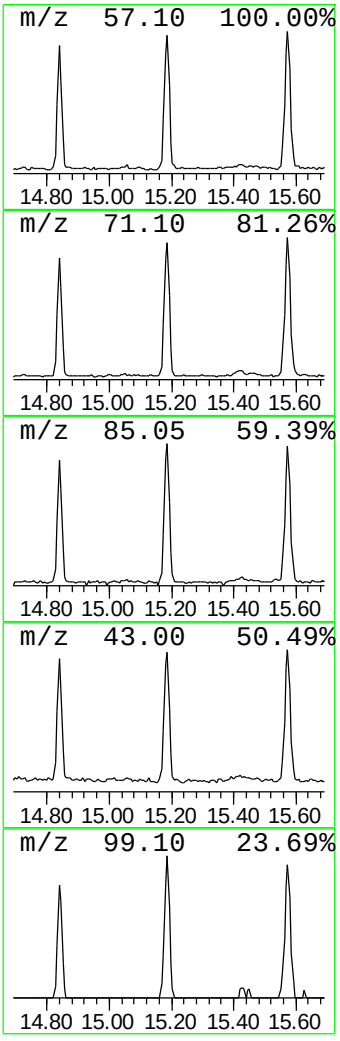
****

Peak Number 7 Triacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.19	3.19 ng	168344	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Heneicosane	296	C21H44	000629-94-7	91





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Instrument : BNA_F
ClientSampleId : HW-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.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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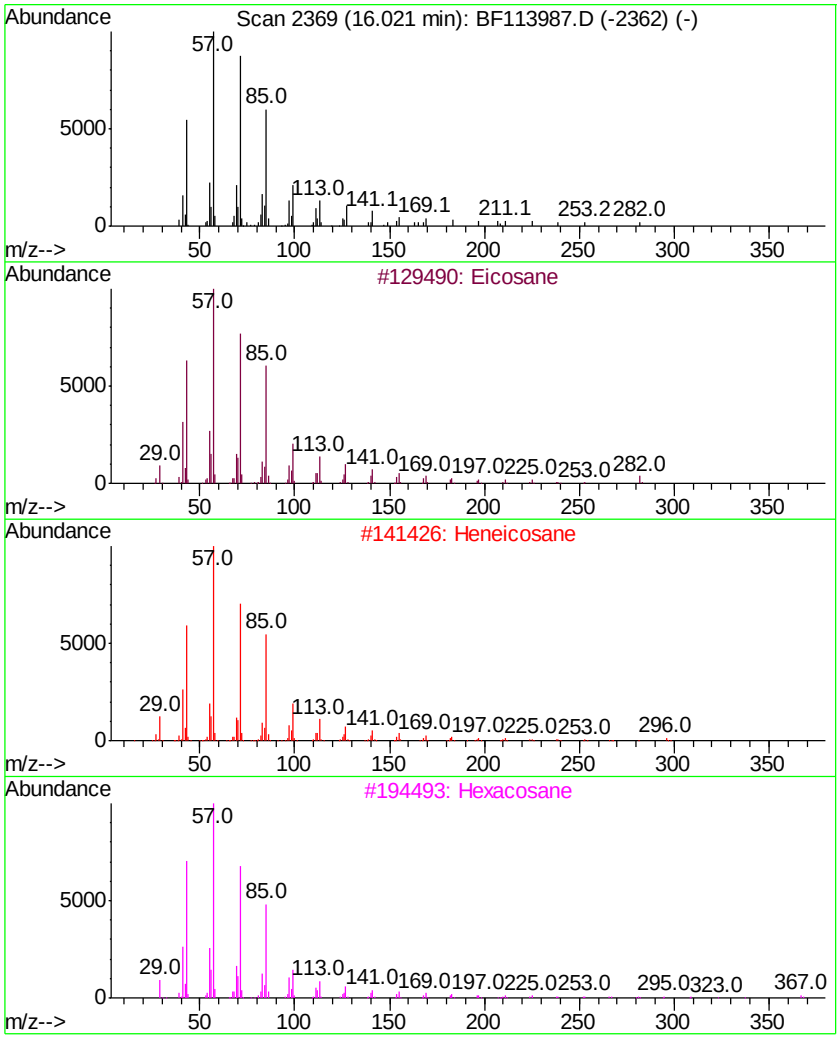
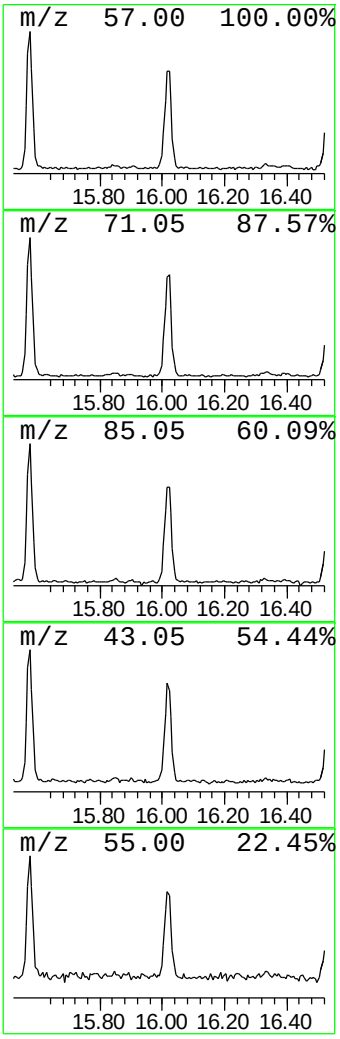
Peak Number 8 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	3.18 ng	168137	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Heneicosane	296	C21H44	000629-94-7	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Triacontane	422	C30H62	000638-68-6	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HW-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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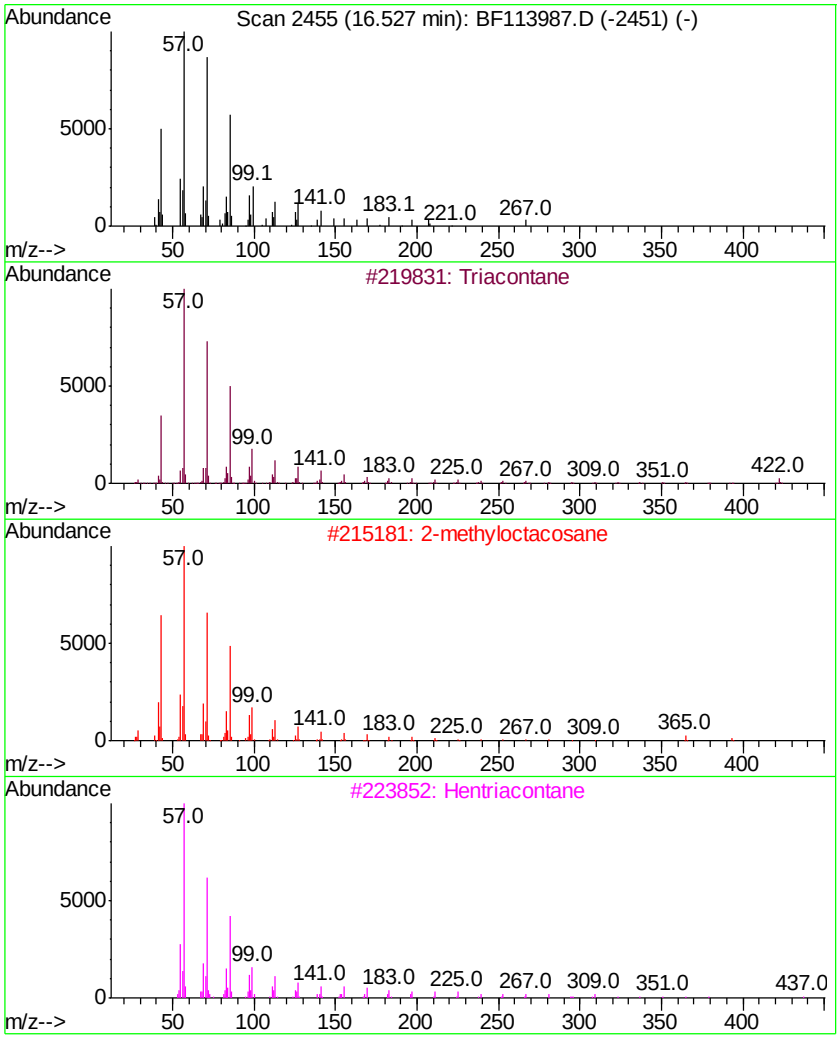
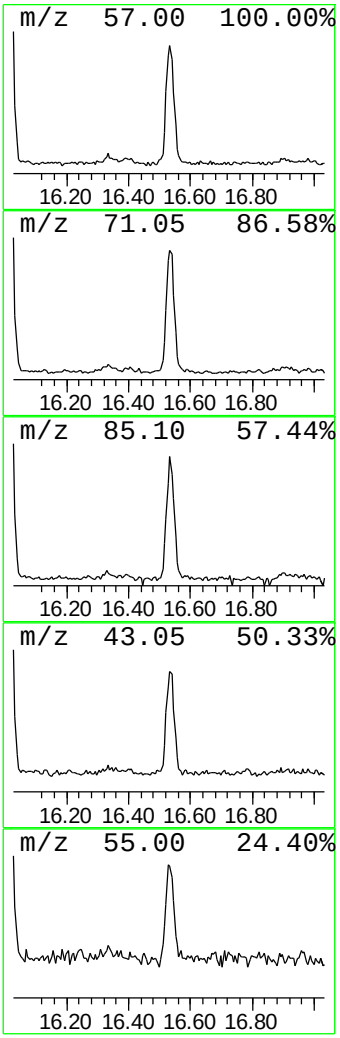
Peak Number 9 Hentriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	2.11 ng	111623	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Hentriacontane	437	C31H64	000630-04-6	90
4	Octacosane	394	C28H58	000630-02-4	87
5	Hexacosane	366	C26H54	000630-01-3	87





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_F
ClientSampleId : HW-15

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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...	2.15	7.7	ng	204591	1	6.89	533367	20.0
unknown6.66	6.66	81.0	ng	2158780	1	6.89	533367	20.0
n-Hexadecanoic acid	11.94	3.9	ng	191488	4	11.42	990953	20.0
Octadecanoic acid	12.72	2.9	ng	143957	4	11.42	990953	20.0
Heptadecane, 9-oc...	14.84	2.4	ng	124929	6	15.54	1056900	20.0
Triacontane	15.19	3.2	ng	168344	6	15.54	1056900	20.0
Eicosane	16.02	3.2	ng	168137	6	15.54	1056900	20.0
Hentriacontane	16.53	2.1	ng	111623	6	15.54	1056900	20.0