LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042519\
Data File : BF113989.D
Acq On : 25 Apr 2019 20:28
Operator : JU/SJ
Sample : K2555-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BLIND-DUPLICATE

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	2.157	6	12	18	rBV	172855	219358	4.75%	0.857%
2	5.510	578	582	600	rBV	1200579	1180676	25.55%	4.614%
3	6.516	749	753	767	rBV	1016622	872263	18.88%	3.409%
4	6.663	774	778	782	rBV	2459216	2240980	48.49%	8.758%
5	6.892	814	817	821	rBV	693869	572167	12.38%	2.236%
6	7.051	840	844	848	rBV	2411409	2159539	46.73%	8.440%
7	7.451	907	912	915	rBV	1749458	1665508	36.04%	6.509%
8	8.175	1032	1035	1047	rBV	773337	725386	15.70%	2.835%
9	9.251	1214	1218	1221	rBV	3931208	3449108	74.64%	13.479%
10	9.933	1330	1334	1346	rVB	939360	910997	19.71%	3.560%
11	10.722	1463	1468	1483	rBV	2273867	2469621	53.44%	9.651%
12	11.416	1582	1586	1594	rBV	1190280	1050026	22.72%	4.104%
13	11.939	1671	1675	1683	rBV2	141376	147361	3.19%	0.576%
14	12.721	1805	1808	1816	rBV	61496	73098	1.58%	0.286%
15	13.004	1851	1856	1859	rBV	4361077	4621145	100.00%	18.060%
16	14.051	2030	2034	2046	rVB	1283314	1202710	26.03%	4.700%
17	14.527	2110	2115	2118	rBV2	88896	89871	1.94%	0.351%
18	14.839	2164	2168	2173	rVB	126414	131811	2.85%	0.515%
19	15.180	2222	2226	2233	rVB	166477	177461	3.84%	0.694%
20	15.539	2281	2287	2290	rBV	773454	1101291	23.83%	4.304%
21	15.568	2290	2292	2300	rVB	183917	204055	4.42%	0.797%
22	16.015	2362	2368	2373	rBV	111677	164606	3.56%	0.643%
23	16.527	2449	2455	2463	rVB3	65608	111432	2.41%	0.435%
24	17.133	2553	2558	2565	rVB2	24943	47881	1.04%	0.187%

Sum of corrected areas: 25588351

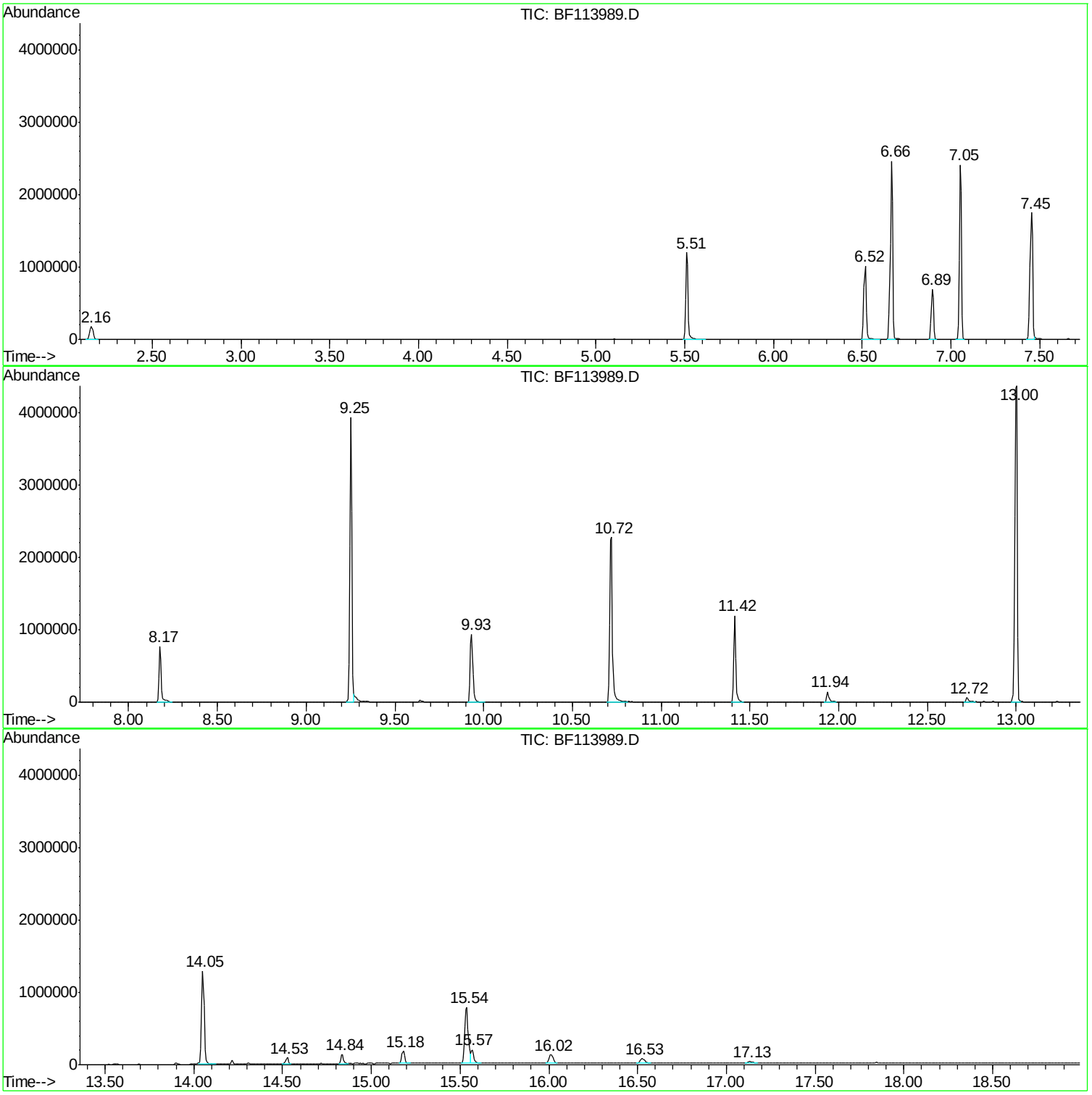
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042519\
Data File : BF113989.D
Acq On : 25 Apr 2019 20:28
Operator : JU/SJ
Sample : K2555-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BLIND-DUPLICATE

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

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042519\
Data File : BF113989.D
Acq On : 25 Apr 2019 20:28
Operator : JU/SJ
Sample : K2555-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BLIND-DUPLICATE

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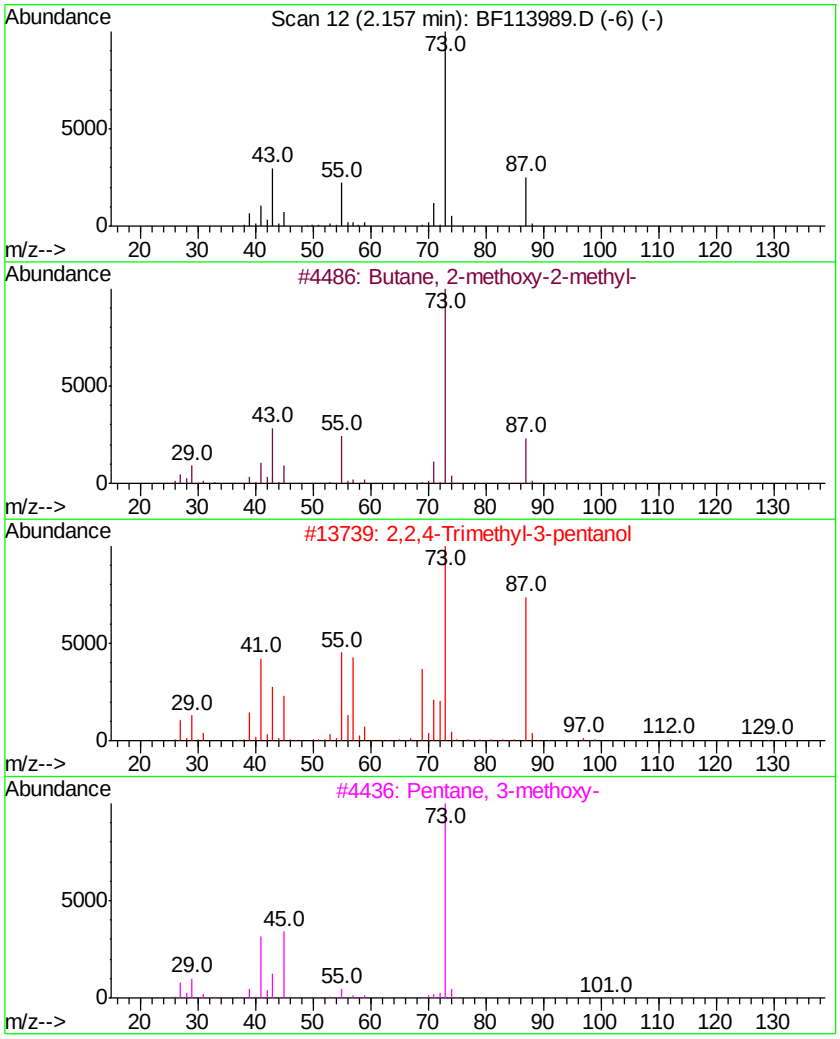
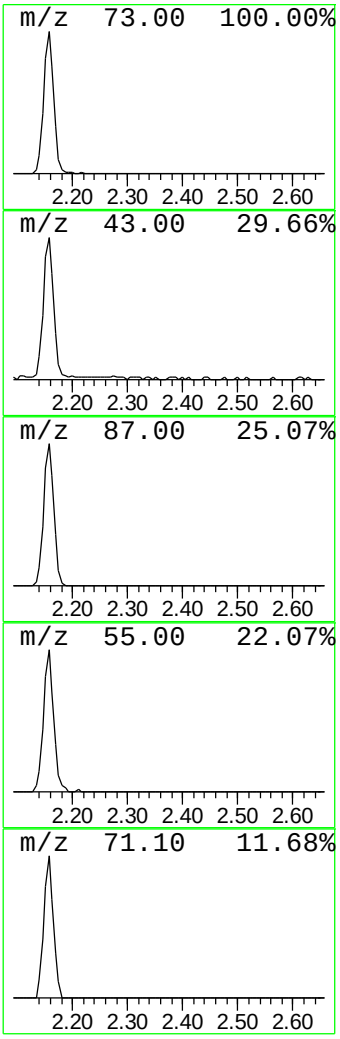
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	7.67 ng	219358	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	43
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Data File : BF113989.D
Acq On : 25 Apr 2019 20:28
Operator : JU/SJ
Sample : K2555-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BLIND-DUPLICATE

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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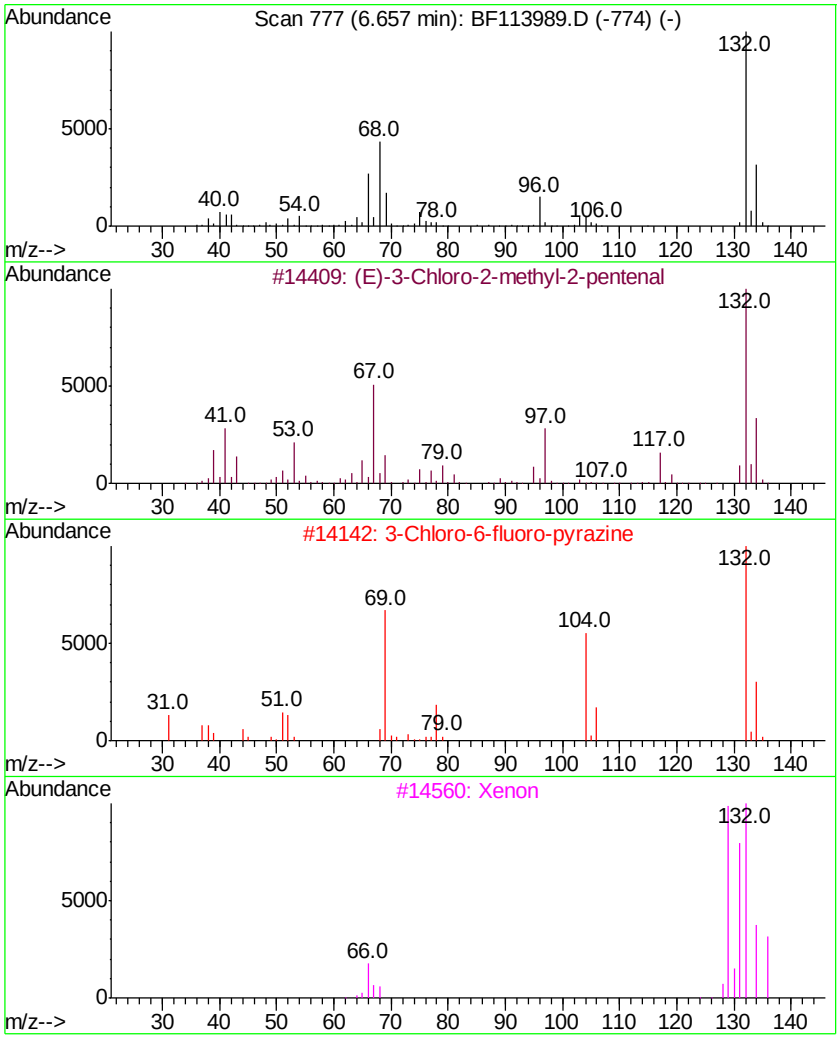
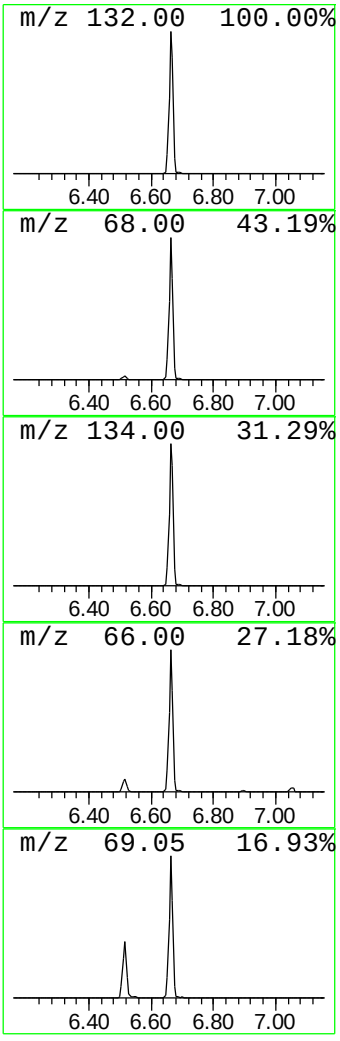
Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	78.33 ng	2240980	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	Xenon	132	Xe	007440-63-3	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042519\
Data File : BF113989.D
Acq On : 25 Apr 2019 20:28
Operator : JU/SJ
Sample : K2555-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BLIND-DUPLICATE

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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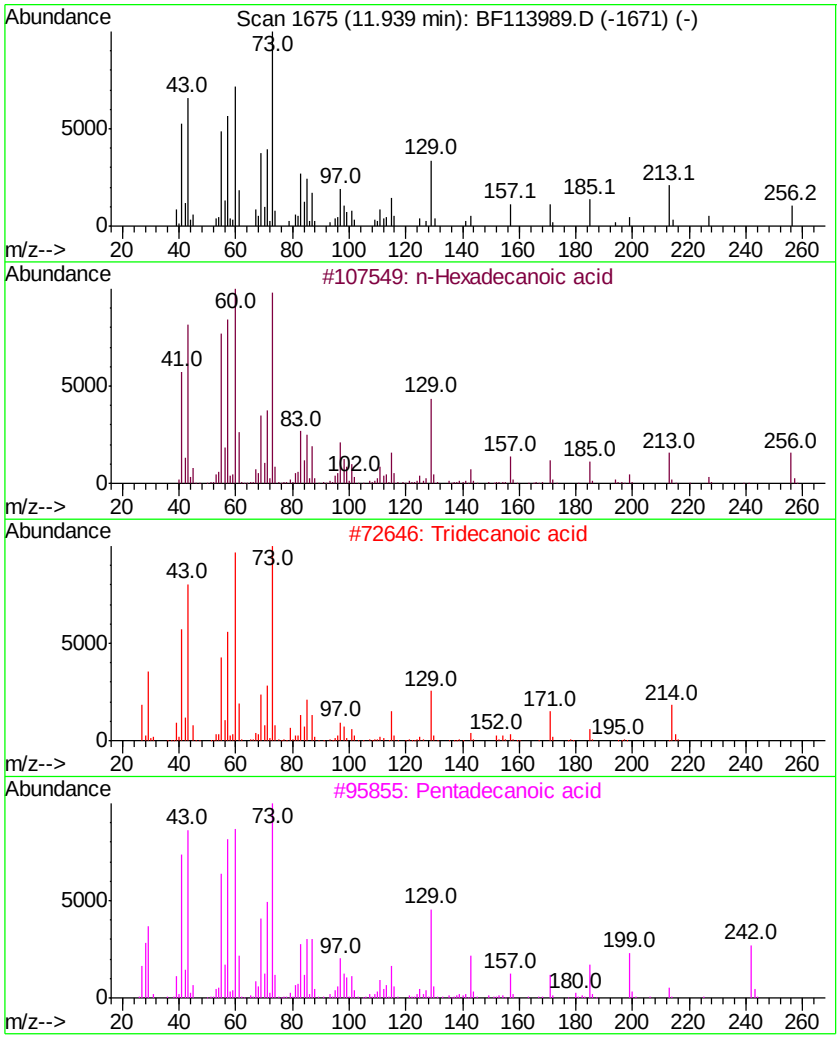
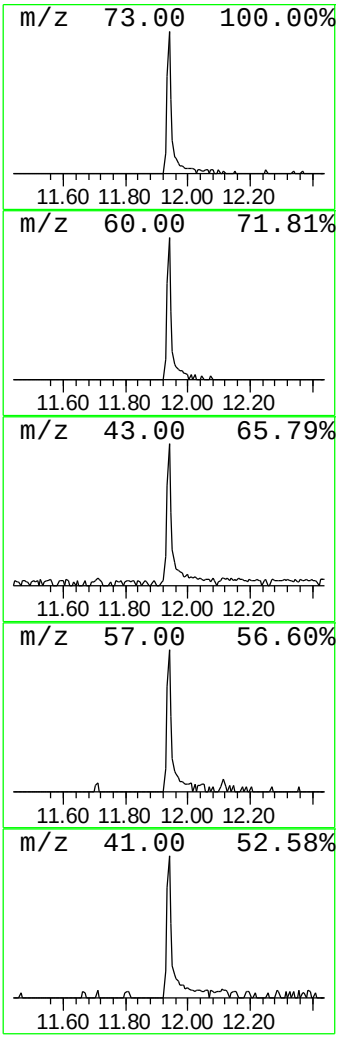
Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	2.81 ng	147361	Phenanthrene-d10	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	78
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	30
5	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	30





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042519\
Data File : BF113989.D
Acq On : 25 Apr 2019 20:28
Operator : JU/SJ
Sample : K2555-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BLIND-DUPLICATE

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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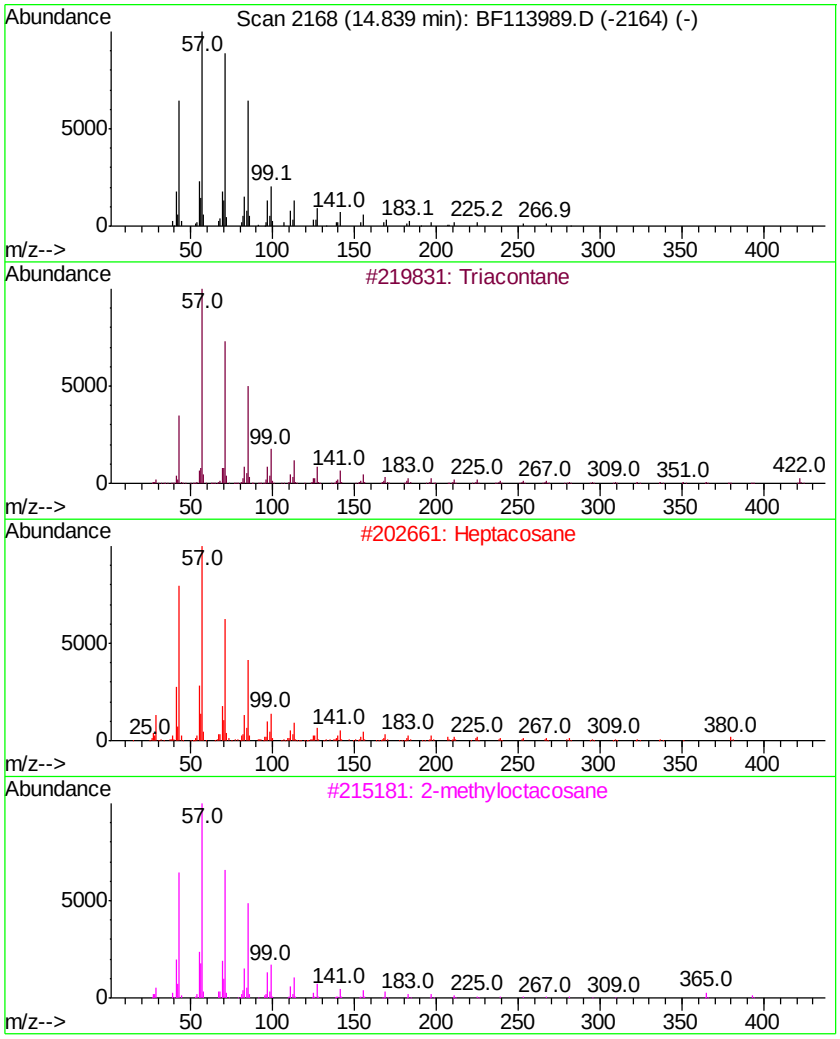
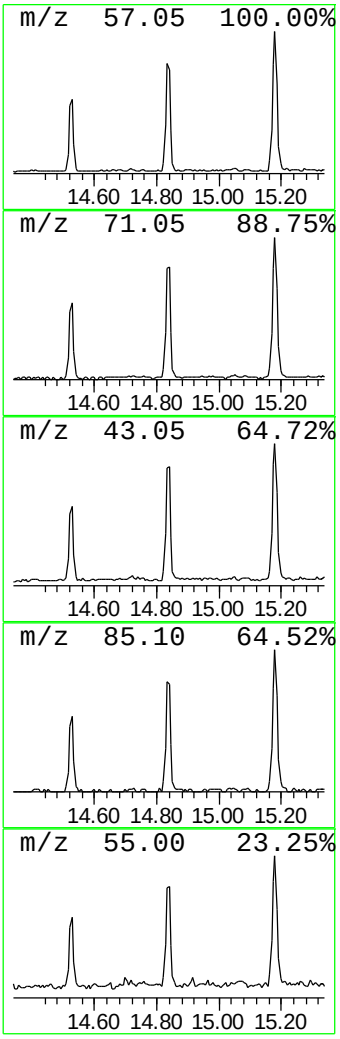
Peak Number 5 Triacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	2.39 ng	131811	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042519\
Data File : BF113989.D
Acq On : 25 Apr 2019 20:28
Operator : JU/SJ
Sample : K2555-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BLIND-DUPLICATE

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

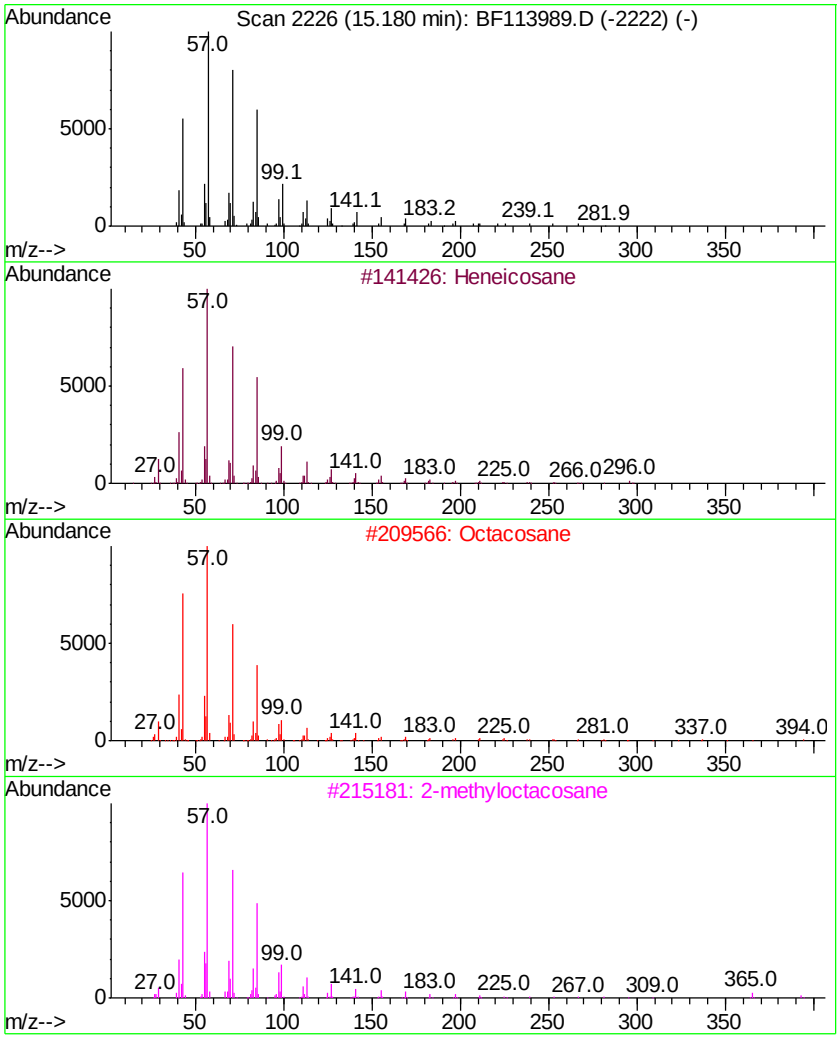
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

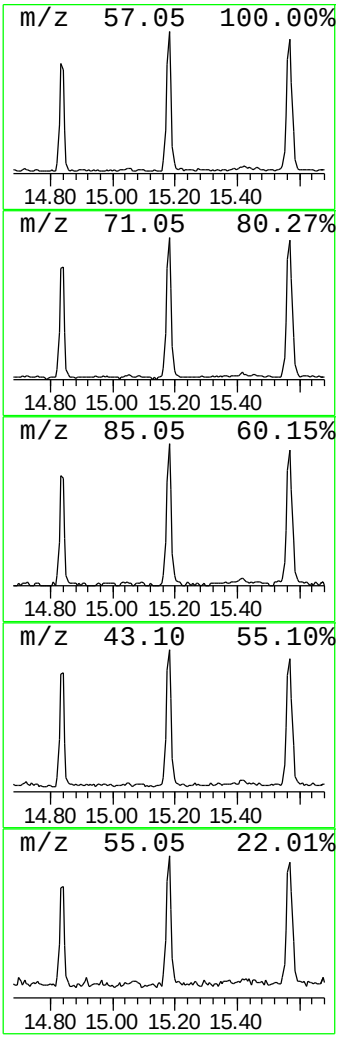
****

Peak Number 6 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.18	3.22 ng	177461	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Triacontane	422	C30H62	000638-68-6	91





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Sample : K2555-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BLIND-DUPLICATE

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

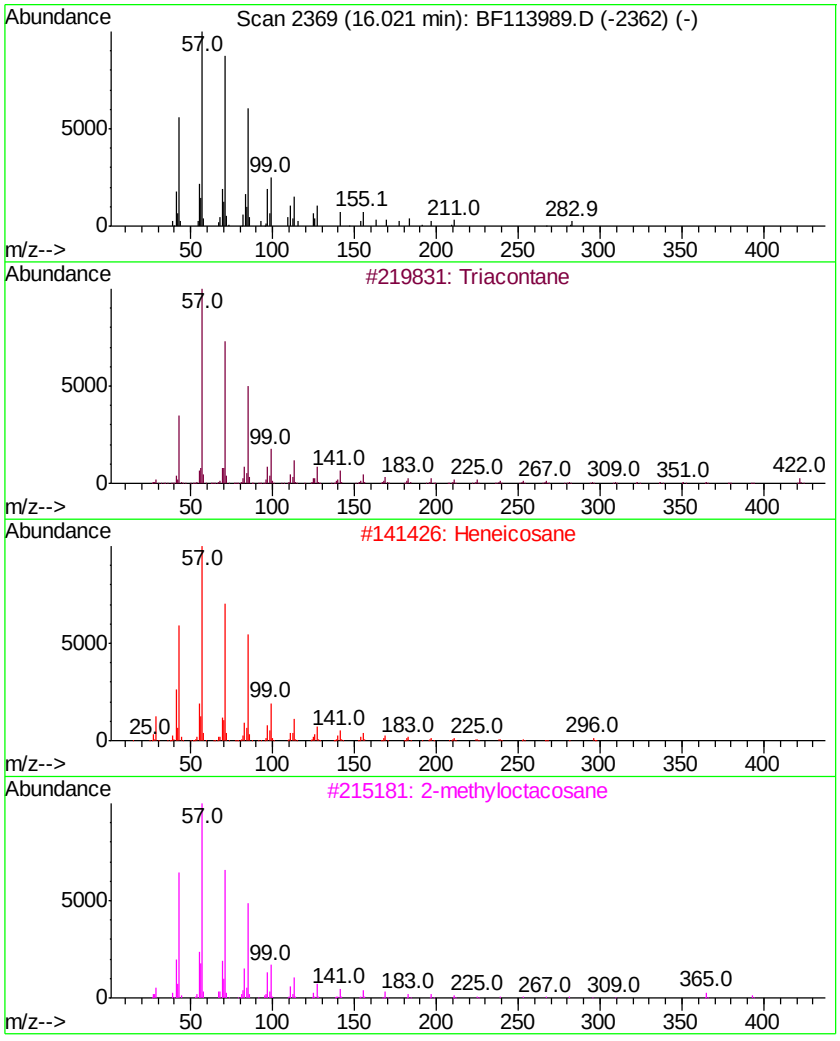
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

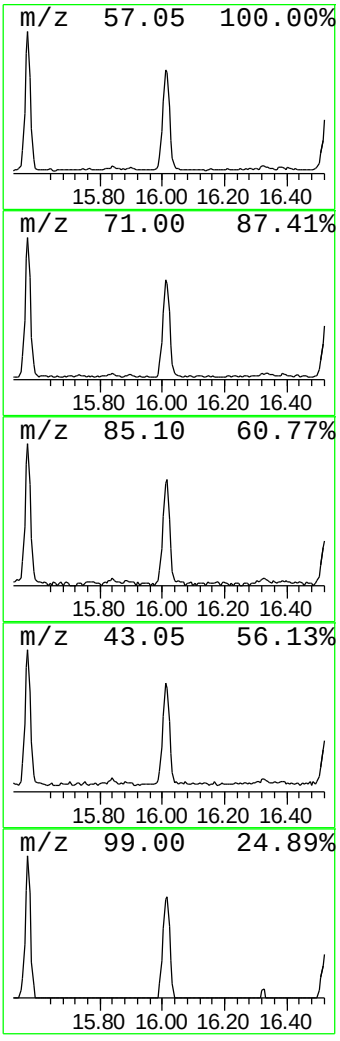
****

Peak Number 7 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	2.99 ng	164606	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Hexacosane	366	C26H54	000630-01-3	91





Library Search Compound Report

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Data File : BF113989.D
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Operator : JU/SJ
Sample : K2555-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BLIND-DUPLICATE

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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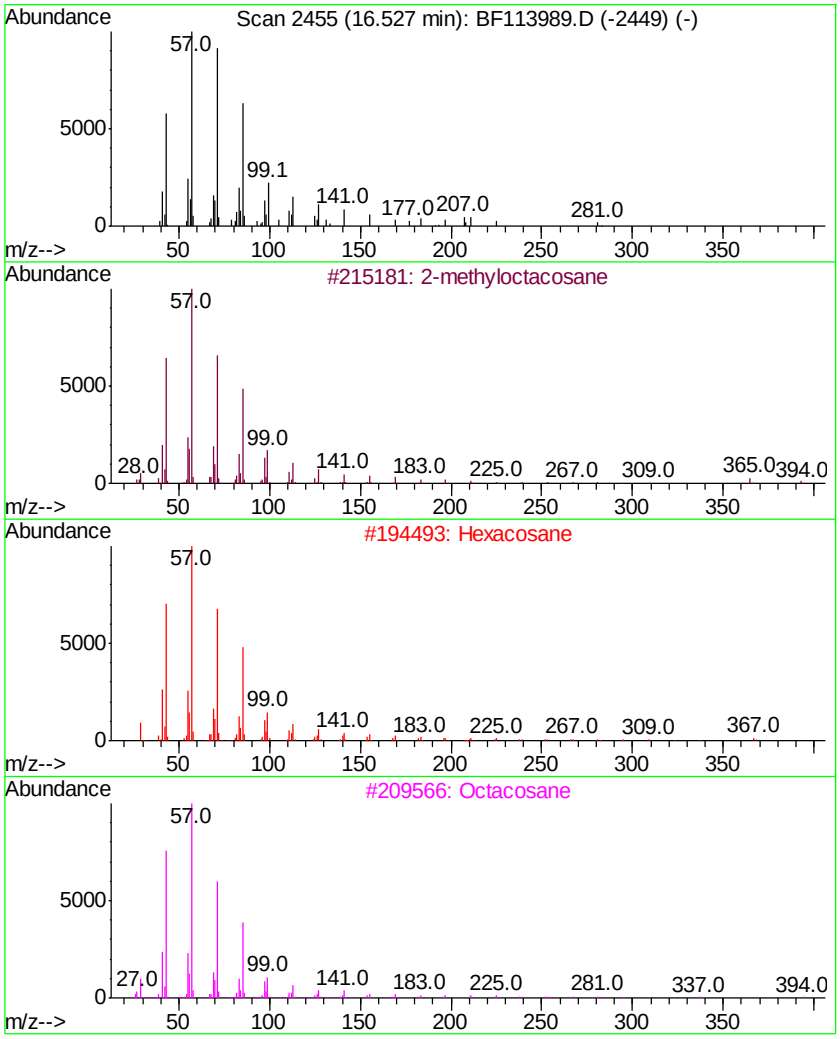
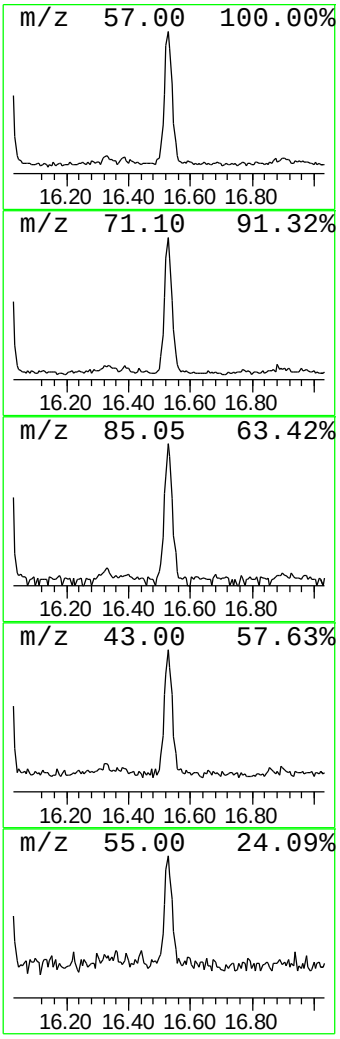
Peak Number 8 2-methyloctacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	2.02 ng	111432	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Heneicosane	296	C21H44	000629-94-7	90
5	Pentacosane	352	C25H52	000629-99-2	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042519\
Data File : BF113989.D
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Operator : JU/SJ
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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
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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...	2.16	7.7	ng	219358	1	6.89	572167	20.0
unknown6.66	6.66	78.3	ng	2240980	1	6.89	572167	20.0
n-Hexadecanoic acid	11.94	2.8	ng	147361	4	11.42	1050030	20.0
Triacontane	14.84	2.4	ng	131811	6	15.54	1101290	20.0
Heneicosane	15.18	3.2	ng	177461	6	15.54	1101290	20.0
Octacosane	16.02	3.0	ng	164606	6	15.54	1101290	20.0
2-methyloctacosane	16.53	2.0	ng	111432	6	15.54	1101290	20.0