LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121819\
Data File : BF118271.D
Acq On : 18 Dec 2019 20:58
Operator : JU
Sample : K6357-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PF-03

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-BF120619.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	2.122	3	6	11	rVB	279030	343688	10.09%	1.251%
2	5.069	503	507	521	rVB	365385	481305	14.13%	1.752%
3	5.481	572	577	580	rBV	2747116	2498814	73.38%	9.095%
4	6.492	744	749	765	rBV	2554120	2797501	82.16%	10.182%
5	6.634	768	773	776	rBV	3175022	2911447	85.50%	10.597%
6	6.857	808	811	819	rBV	669220	546274	16.04%	1.988%
7	7.016	834	838	841	rBV	2756631	2263071	66.46%	8.237%
8	7.422	903	907	918	rBV	1605266	1709850	50.21%	6.223%
9	8.145	1026	1030	1047	rBV	755565	696786	20.46%	2.536%
10	9.222	1209	1213	1228	rBV	3394984	3361313	98.71%	12.234%
11	9.622	1277	1281	1291	rBV	155622	155129	4.56%	0.565%
12	9.910	1326	1330	1340	rBV	807891	806711	23.69%	2.936%
13	10.704	1460	1465	1481	rBV	2293635	2321225	68.17%	8.449%
14	11.404	1580	1584	1591	rBV	802781	822390	24.15%	2.993%
15	11.921	1669	1672	1685	rBV	158195	185067	5.44%	0.674%
16	12.716	1804	1807	1815	rBV3	25911	37325	1.10%	0.136%
17	12.992	1849	1854	1857	rBV	3909277	3405091	100.00%	12.394%
18	13.886	2002	2006	2024	rBV	260450	392091	11.51%	1.427%
19	14.057	2031	2035	2045	rBV	597348	640583	18.81%	2.332%
20	14.204	2056	2060	2067	rBV	46799	49147	1.44%	0.179%
21	14.509	2109	2112	2115	rBV	66147	65857	1.93%	0.240%
22	14.821	2160	2165	2170	rBV	67159	69500	2.04%	0.253%
23	15.162	2220	2223	2229	rBV	66665	81032	2.38%	0.295%
24	15.545	2283	2288	2299	rBV2	450959	666132	19.56%	2.425%
25	15.998	2358	2365	2371	rBV2	49272	75415	2.21%	0.274%
26	16.068	2372	2377	2383	rBV8	20772	48202	1.42%	0.175%
27	16.509	2448	2452	2457	rBV2	24948	43701	1.28%	0.159%

Sum of corrected areas: 27474647

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Misc :
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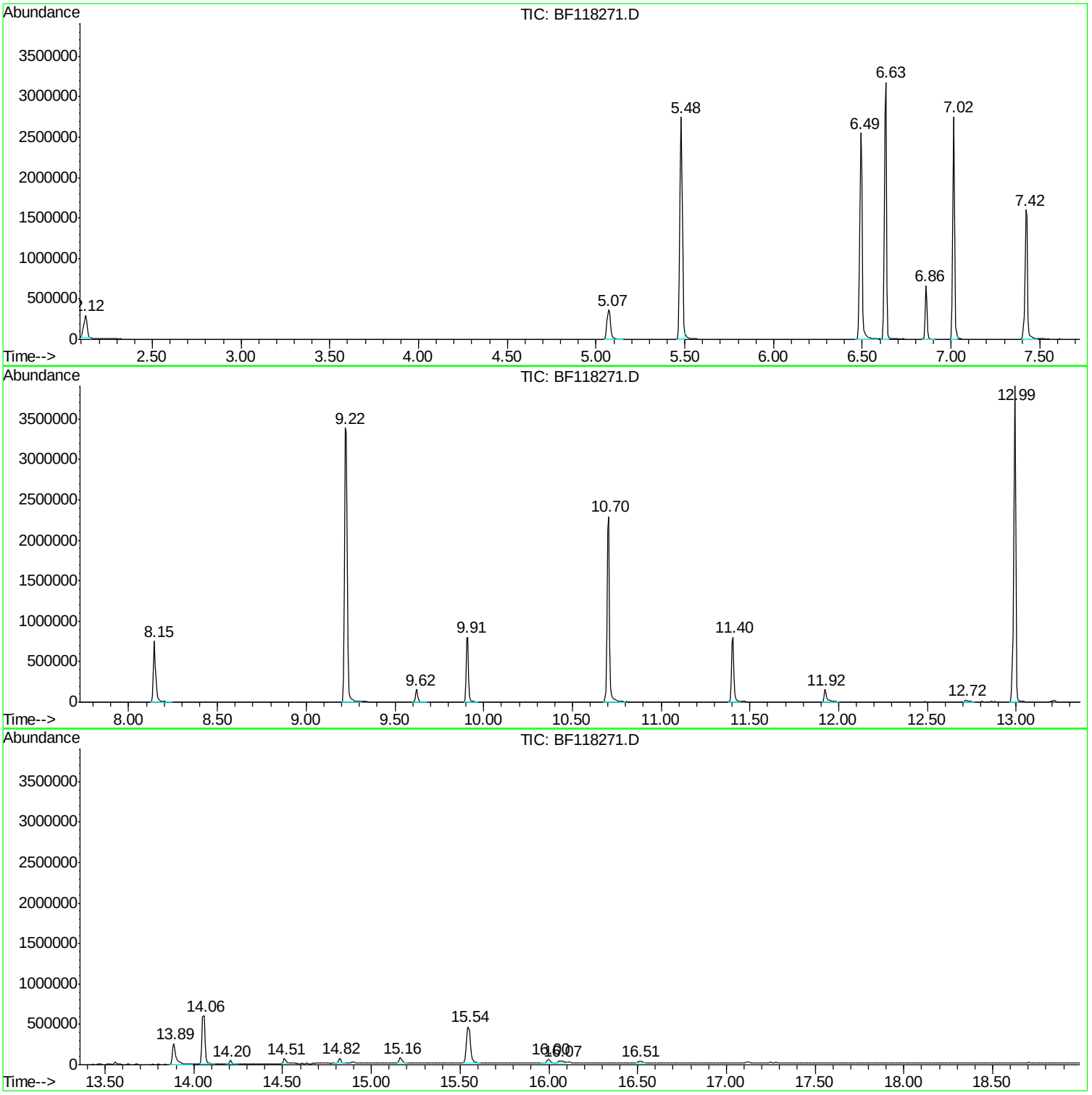
Instrument :
BNA_F
ClientSampleId :
PF-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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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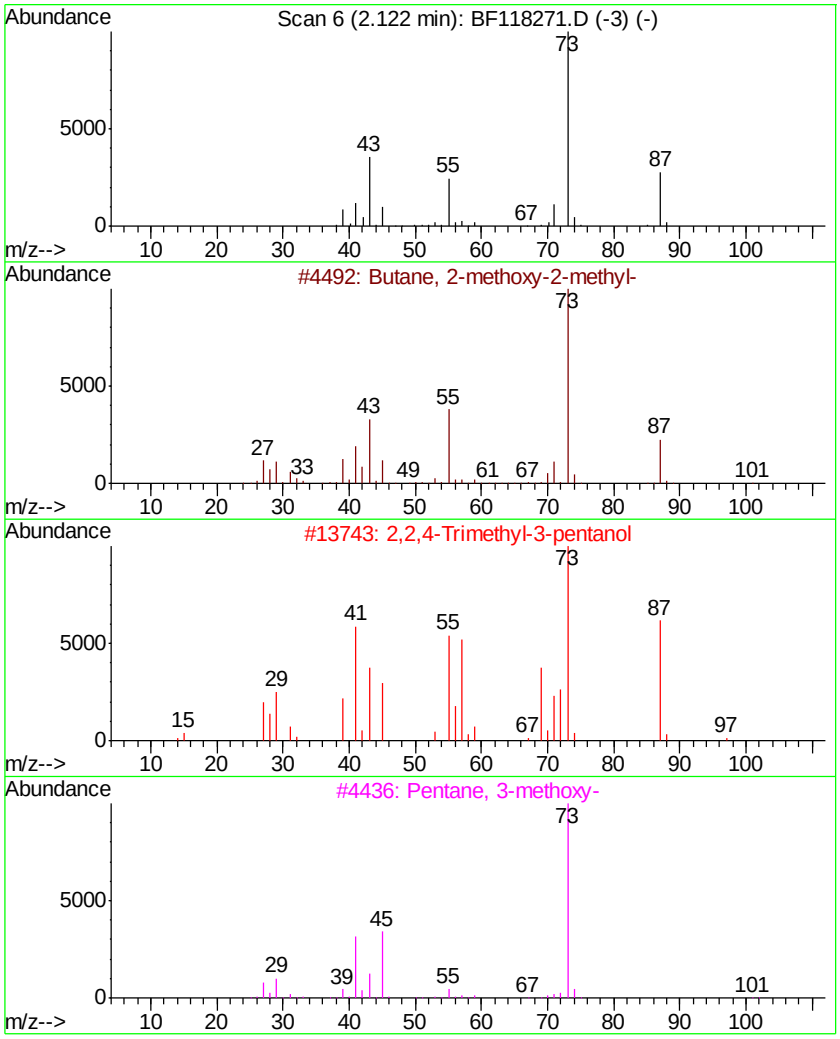
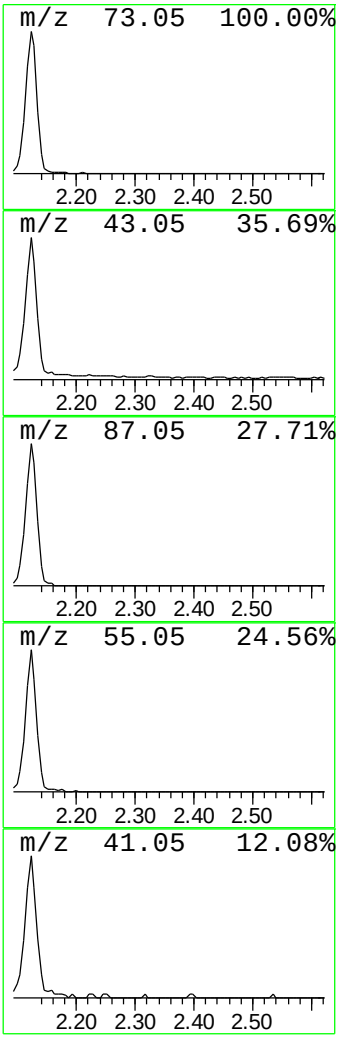
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	12.58 ng	343688	1,4-Dichlorobenzene-d4	6.86

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	56
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	16
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

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Operator : JU
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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PF-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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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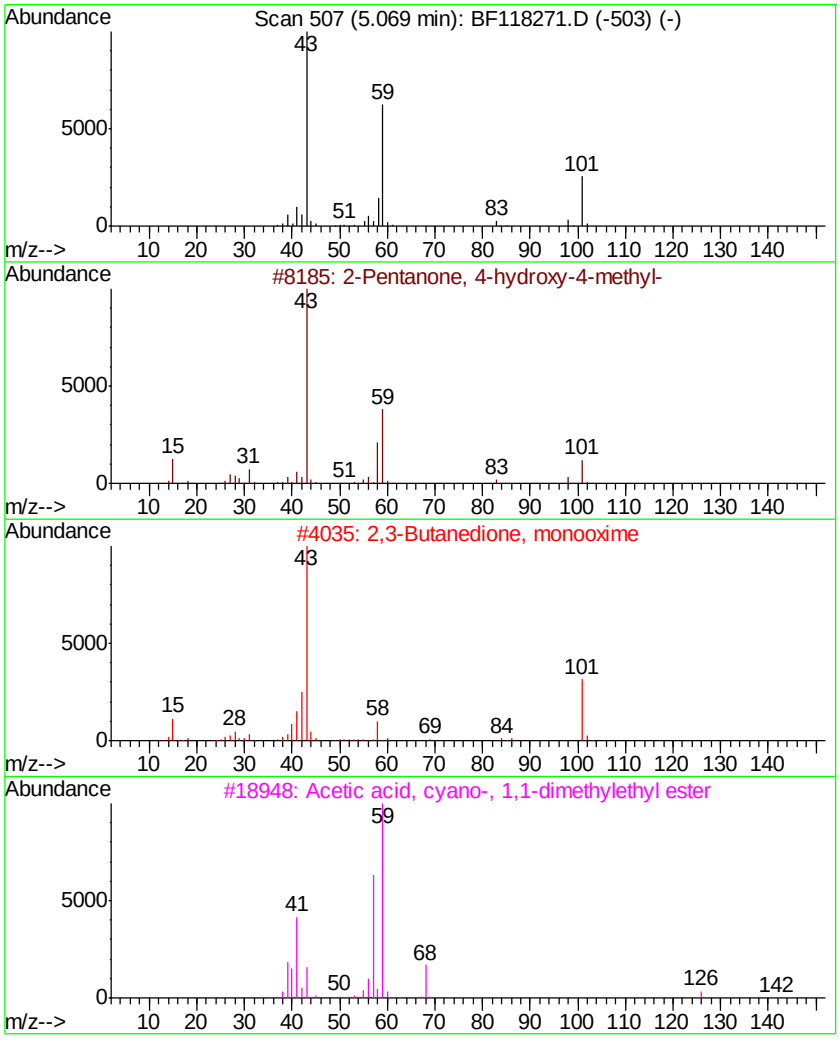
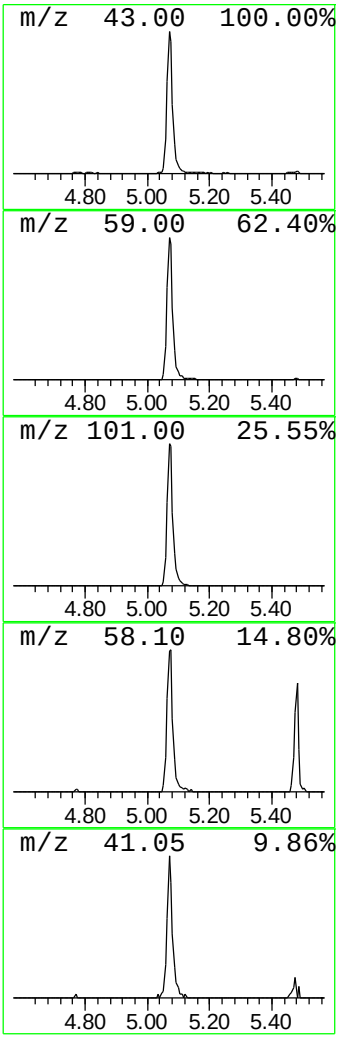
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	17.62 ng	481305	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Butane	58	C4H10	000106-97-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PF-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
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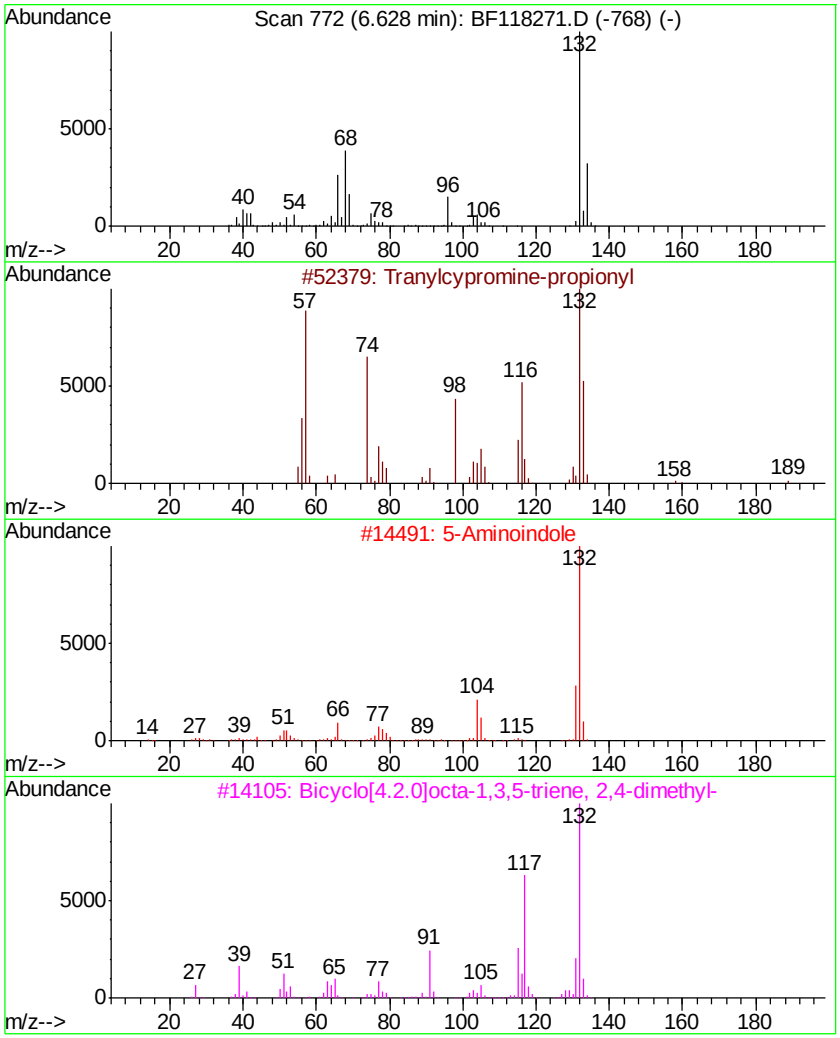
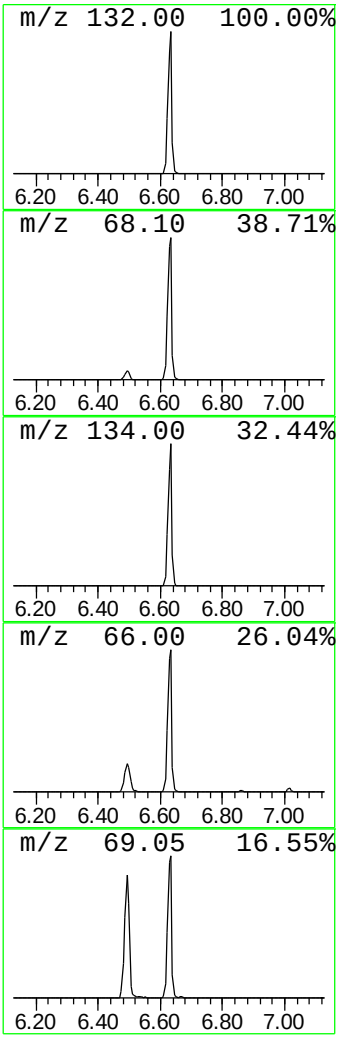
Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	106.59 ng	2911450	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	16
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Xenon	132	Xe	007440-63-3	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PF-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

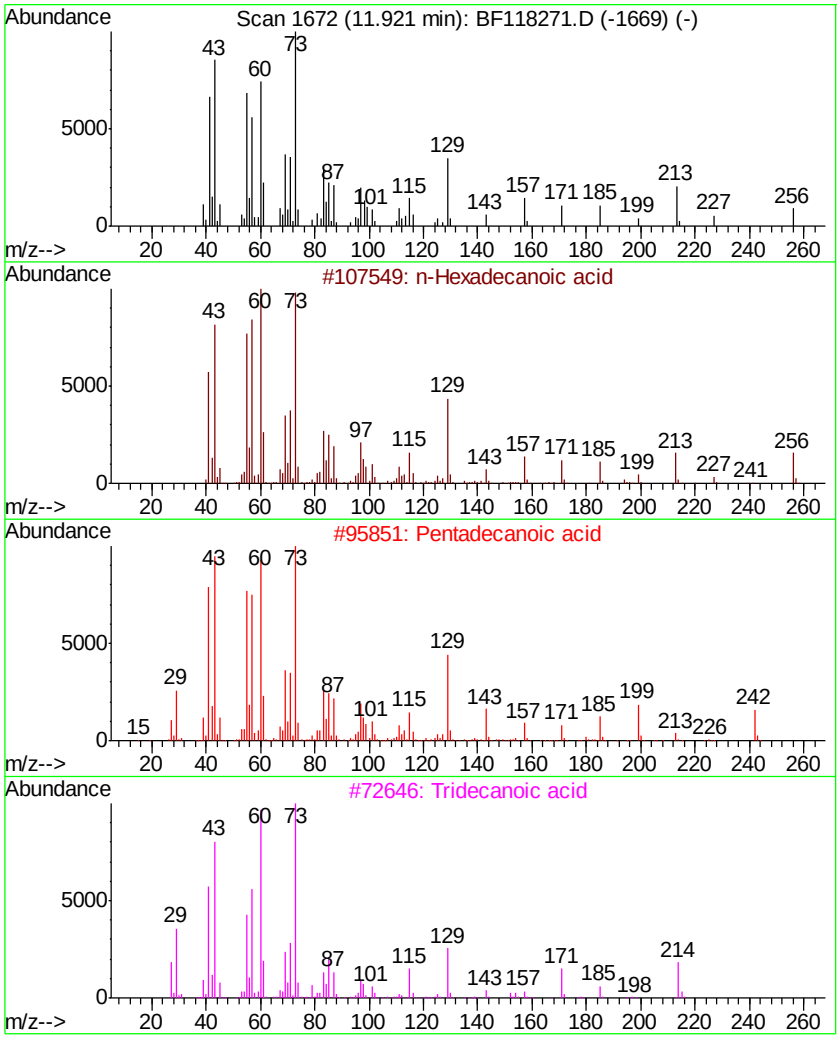
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

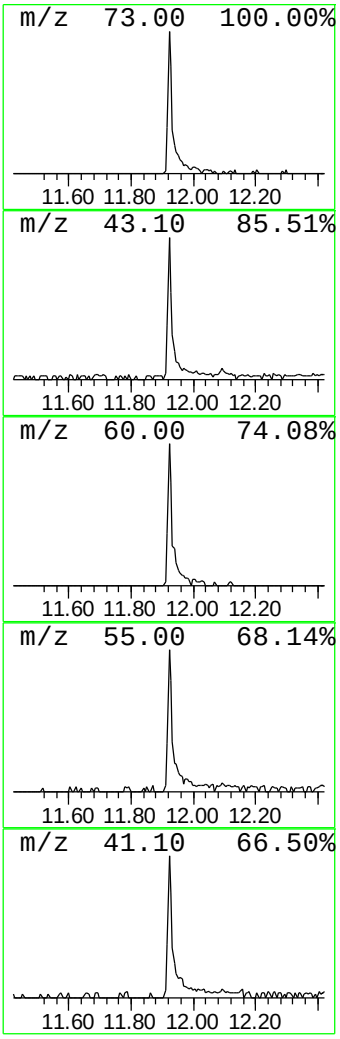
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	4.50 ng	185067	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	70
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Trehalose	342	C12H22O11	000099-20-7	50





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121819\
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Instrument : BNA_F
ClientSampleId : PF-03

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TIC Library : C:\DATABASE\NIST11.L
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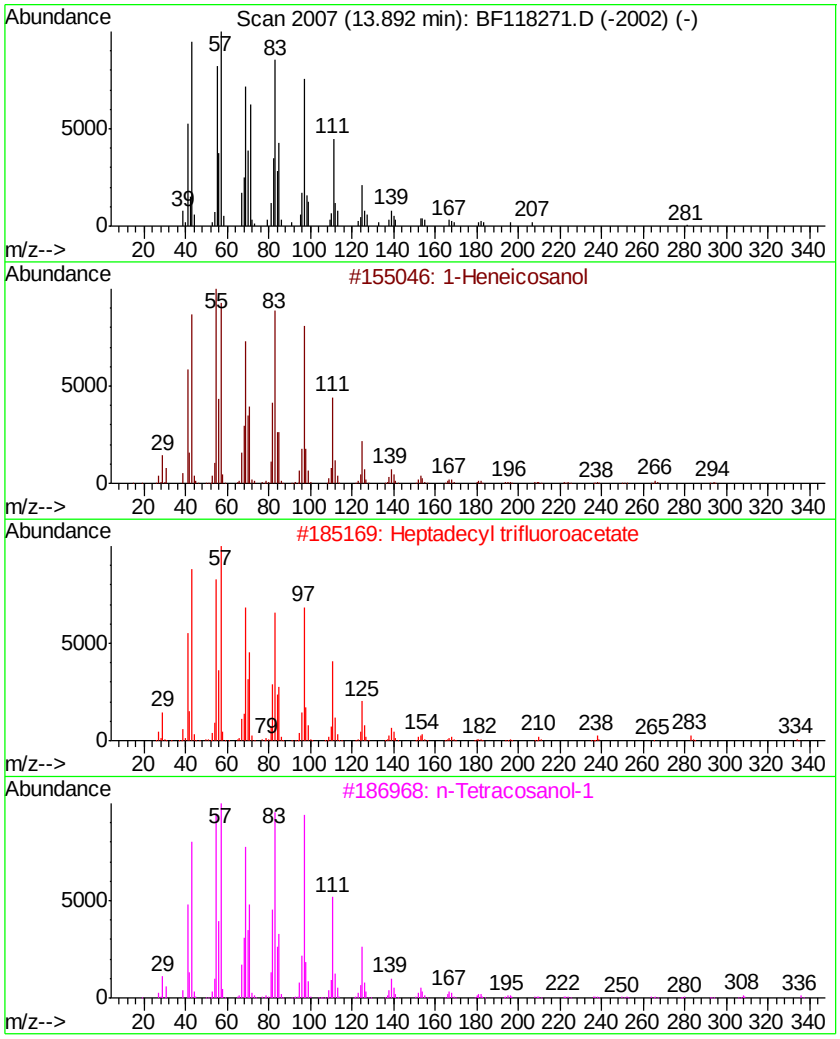
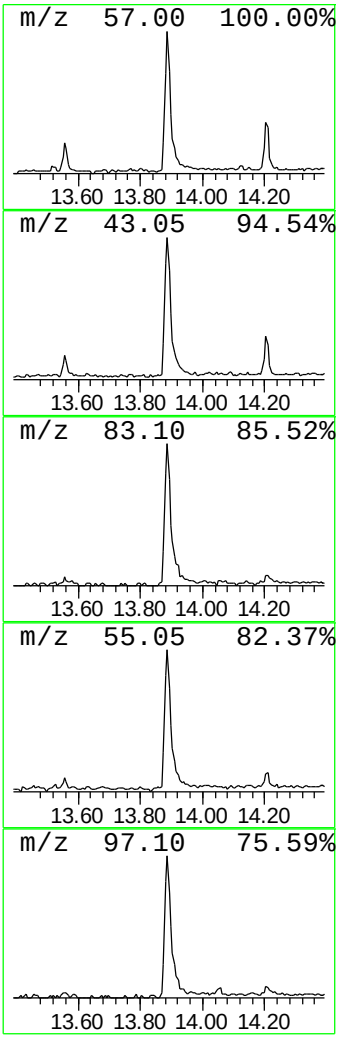
****

Peak Number 6 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	12.24 ng	392091	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	93





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ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PF-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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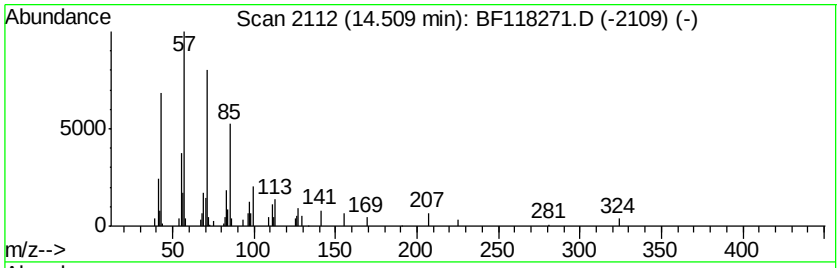
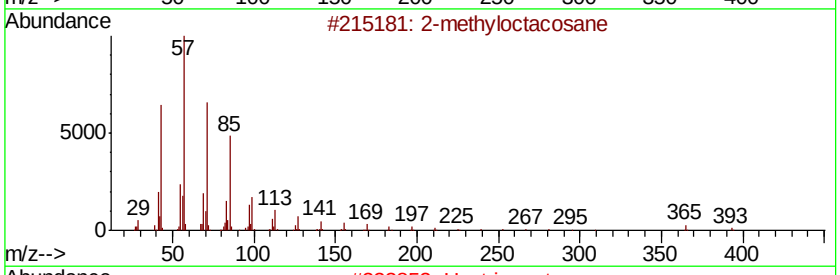
****

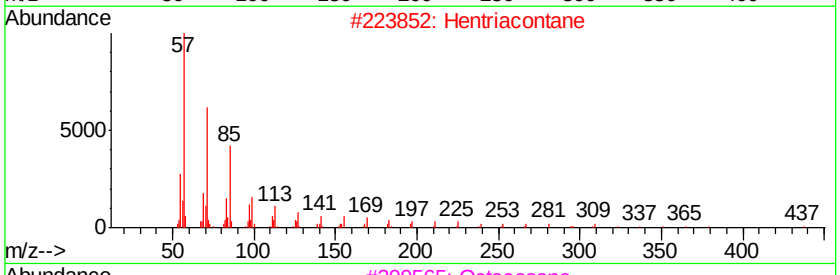
Peak Number 7 2-methyloctacosane Concentration Rank 10

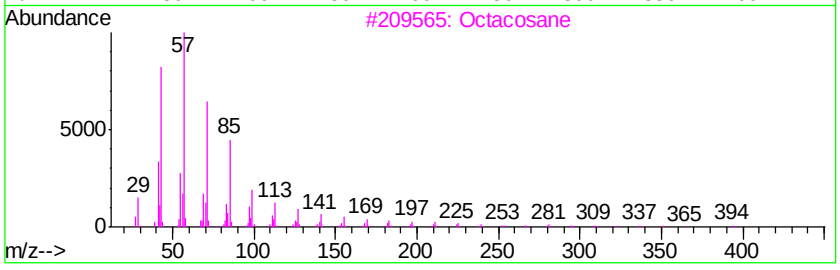
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.51	2.06 ng	65857	Chrysene-d12	14.06

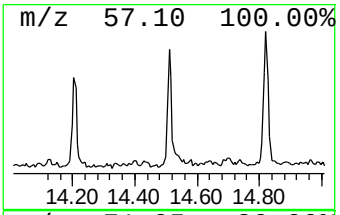
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Hentriacontane	437	C31H64	000630-04-6	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Heptacosane	380	C27H56	000593-49-7	91

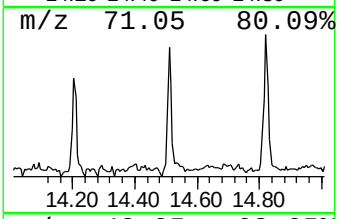


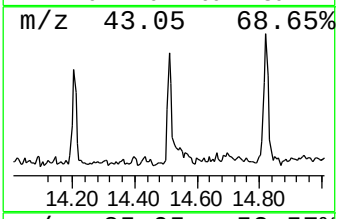


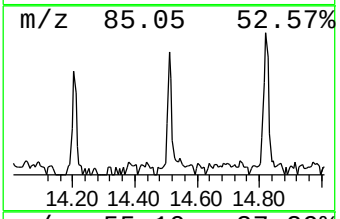


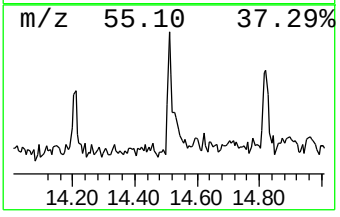












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TIC Library : C:\DATABASE\NIST11.L
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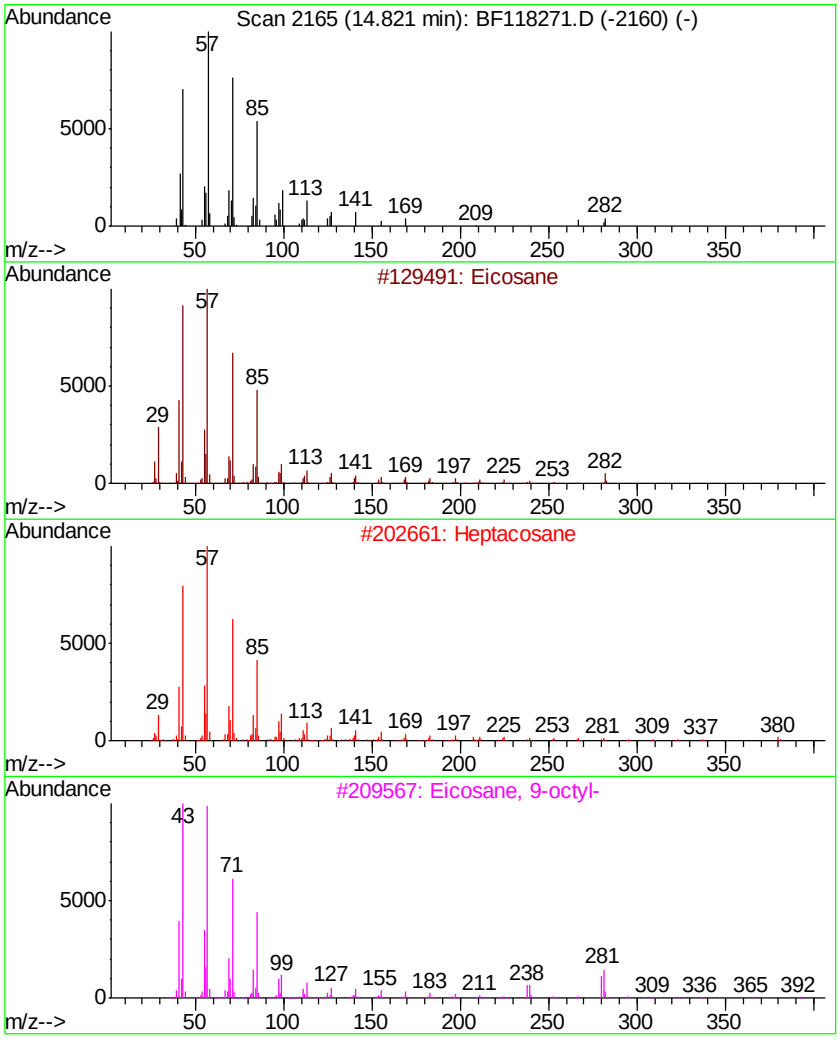
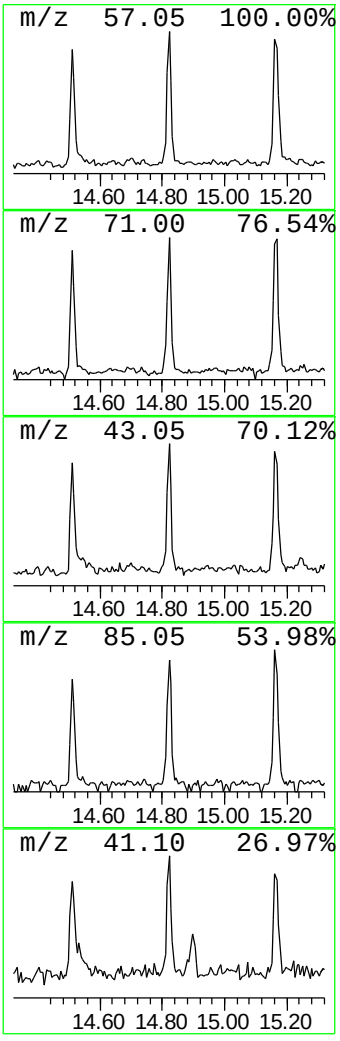
Peak Number 8 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	2.09 ng	69500	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Heptacosane	380	C27H56	000593-49-7	90
3	Eicosane, 9-octyl-	394	C28H58	013475-77-9	90
4	Heptadecane	240	C17H36	000629-78-7	87
5	Heneicosane	296	C21H44	000629-94-7	87





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

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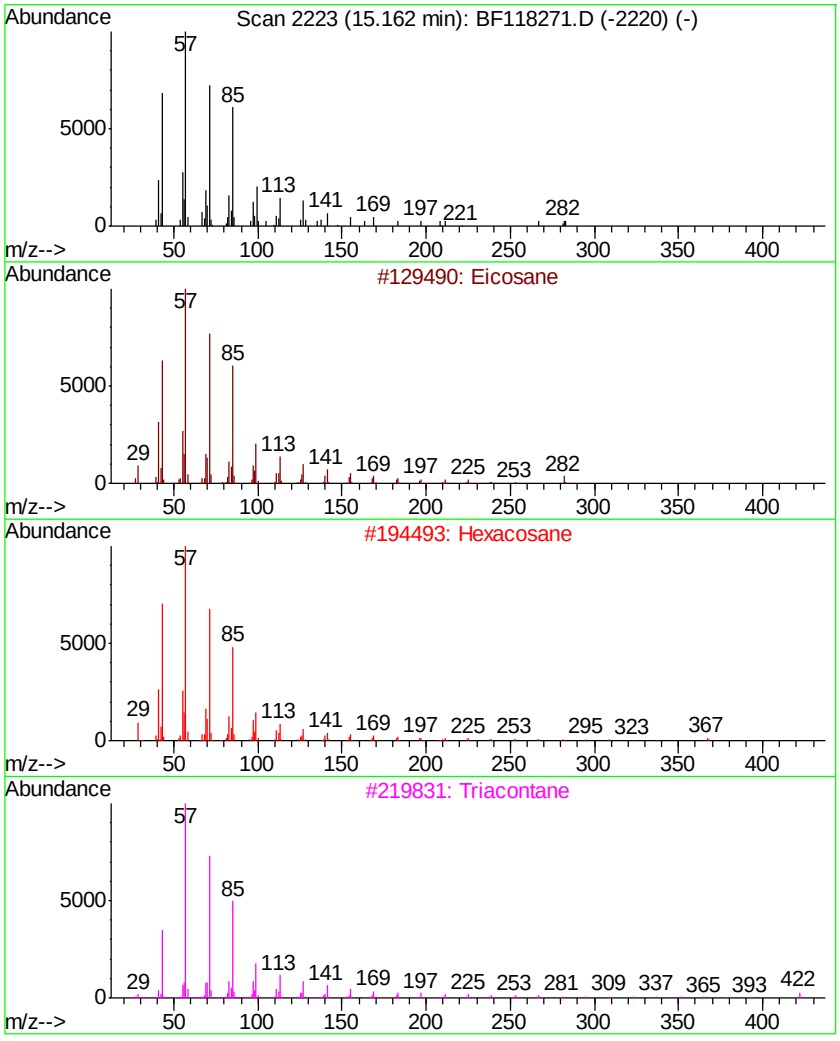
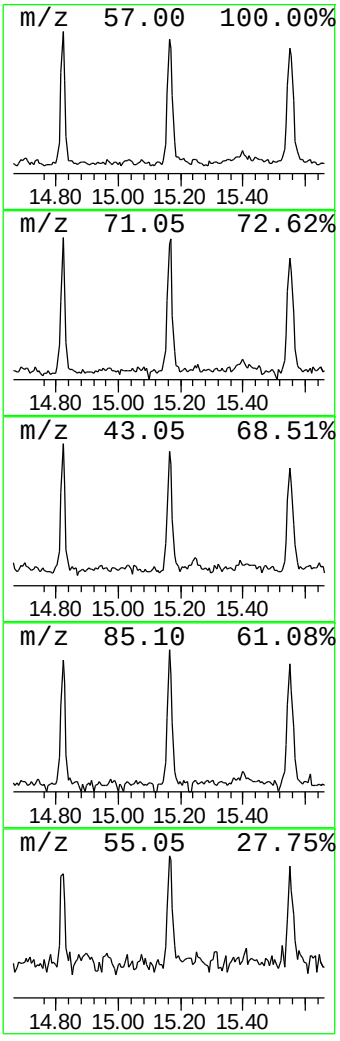
Peak Number 9 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	2.43 ng	81032	Perylene-d12	15.54

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	Triacontane	422	C30H62	000638-68-6	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Heneicosane	296	C21H44	000629-94-7	91





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TIC Integration Parameters: LSCINT.P

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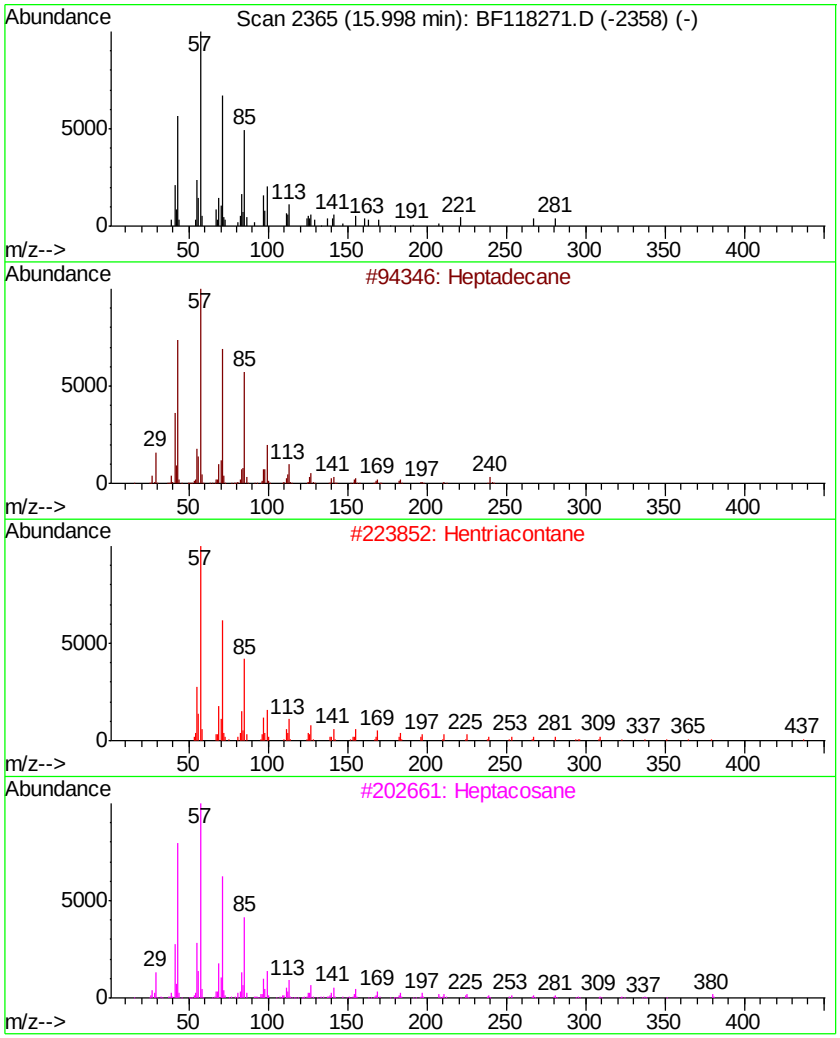
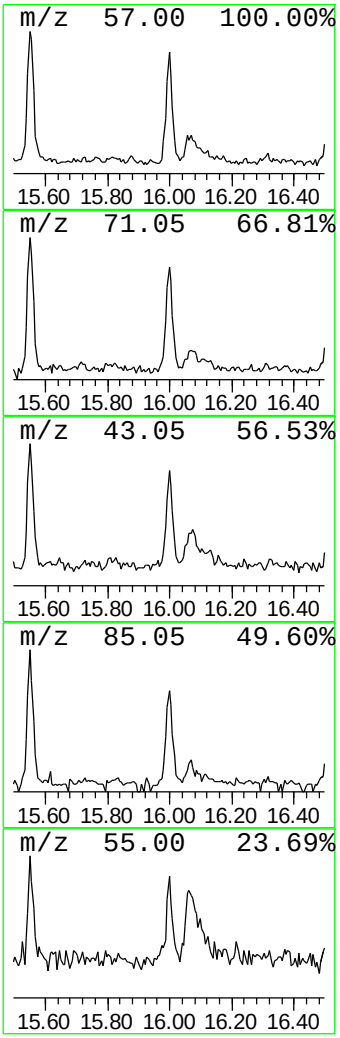
Peak Number 10 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.00	2.26 ng	75415	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	87
2	Hentriacontane	437	C31H64	000630-04-6	87
3	Heptacosane	380	C27H56	000593-49-7	83
4	Heneicosane	296	C21H44	000629-94-7	83
5	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121819\
Data File : BF118271.D
Acq On : 18 Dec 2019 20:58
Operator : JU
Sample : K6357-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PF-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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...	2.12	12.6	ng	343688	1	6.86	546274	20.0
2-Pentanone, 4-hy...	5.07	17.6	ng	481305	1	6.86	546274	20.0
unknown6.63	6.63	106.6	ng	2911450	1	6.86	546274	20.0
n-Hexadecanoic acid	11.92	4.5	ng	185067	4	11.40	822390	20.0
1-Heneicosanol	13.89	12.2	ng	392091	5	14.06	640583	20.0
2-methyloctacosane	14.51	2.1	ng	65857	5	14.06	640583	20.0
Eicosane	14.82	2.1	ng	69500	6	15.54	666132	20.0
Hexacosane	15.16	2.4	ng	81032	6	15.54	666132	20.0
Heptadecane	16.00	2.3	ng	75415	6	15.54	666132	20.0