LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA F\Data\BF122819\
Data File : BF118371.D
Acq On : 28 Dec 2019 18:01
Operator : JU
Sample : K6438-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUNR-BF001-01

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-BF122419.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	5.063	502	506	523	rVB	464563	600746	12.70%	1.753%
2	5.475	572	576	596	rBV	2968763	2923419	61.80%	8.532%
3	6.492	744	749	767	rBV	2915849	3192258	67.48%	9.316%
4	6.628	767	772	775	rBV	3459826	3336300	70.52%	9.737%
5	6.851	806	810	817	rBV	784465	641666	13.56%	1.873%
6	7.010	833	837	840	rBV	2899282	2541209	53.72%	7.416%
7	7.416	902	906	923	rBV	1888014	1940853	41.03%	5.664%
8	8.139	1025	1029	1047	rBV	831836	821255	17.36%	2.397%
9	9.216	1208	1212	1227	rBV	4467152	3937546	83.23%	11.491%
10	9.616	1276	1280	1290	rVB	107148	112843	2.39%	0.329%
11	9.898	1324	1328	1338	rBV	1075923	989856	20.92%	2.889%
12	10.692	1459	1463	1479	rBV	2642117	2849584	60.24%	8.316%
13	11.392	1578	1582	1591	rBV	1114693	1065737	22.53%	3.110%
14	11.916	1667	1671	1686	rBV	369205	404628	8.55%	1.181%
15	12.704	1802	1805	1814	rBV2	76704	106370	2.25%	0.310%
16	12.986	1848	1853	1856	rBV	5324157	4730726	100.00%	13.806%
17	13.874	2000	2004	2022	rBV	565382	773611	16.35%	2.258%
18	14.045	2029	2033	2041	rBV	1029479	1019155	21.54%	2.974%
19	14.192	2054	2058	2067	rBV	72468	93875	1.98%	0.274%
20	14.498	2107	2110	2112	rBV	117530	133145	2.81%	0.389%
21	14.515	2112	2113	2124	rVB	117265	166495	3.52%	0.486%
22	14.809	2157	2163	2167	rBV2	141528	171892	3.63%	0.502%
23	15.151	2216	2221	2225	rBV	149058	165367	3.50%	0.483%
24	15.539	2282	2287	2297	rVB	777270	1060479	22.42%	3.095%
25	15.980	2356	2362	2368	rBV	98760	160535	3.39%	0.469%
26	16.051	2368	2374	2386	rVB4	70790	199967	4.23%	0.584%
27	16.492	2444	2449	2453	rBV3	43045	71888	1.52%	0.210%
28	17.215	2565	2572	2577	rBV3	19255	54233	1.15%	0.158%

Sum of corrected areas: 34265638

Data Path : Z:\svoasrv\HPCHEM1\BNA F\Data\BF122819\
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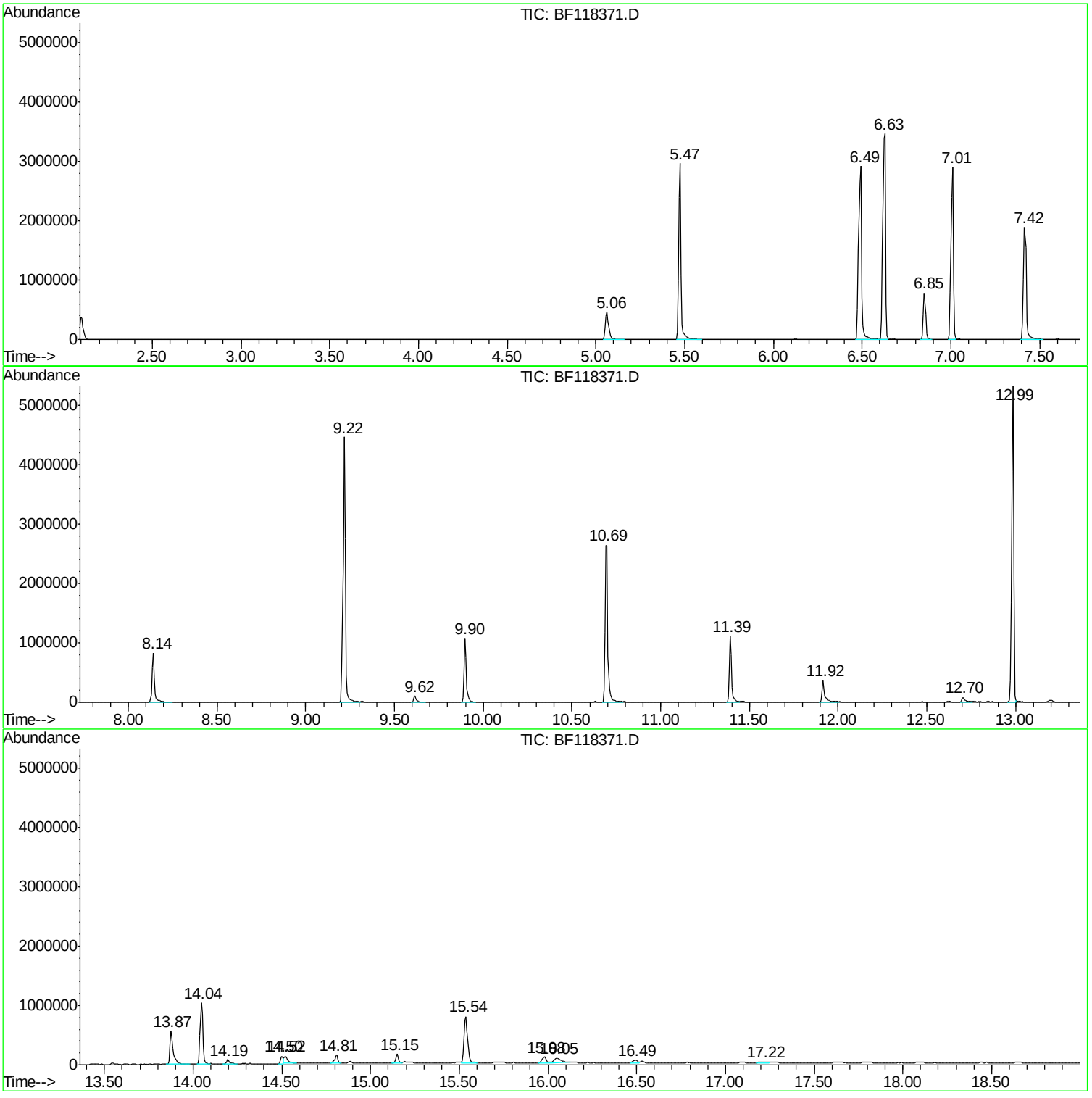
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUNR-BF001-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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\BF122819\
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

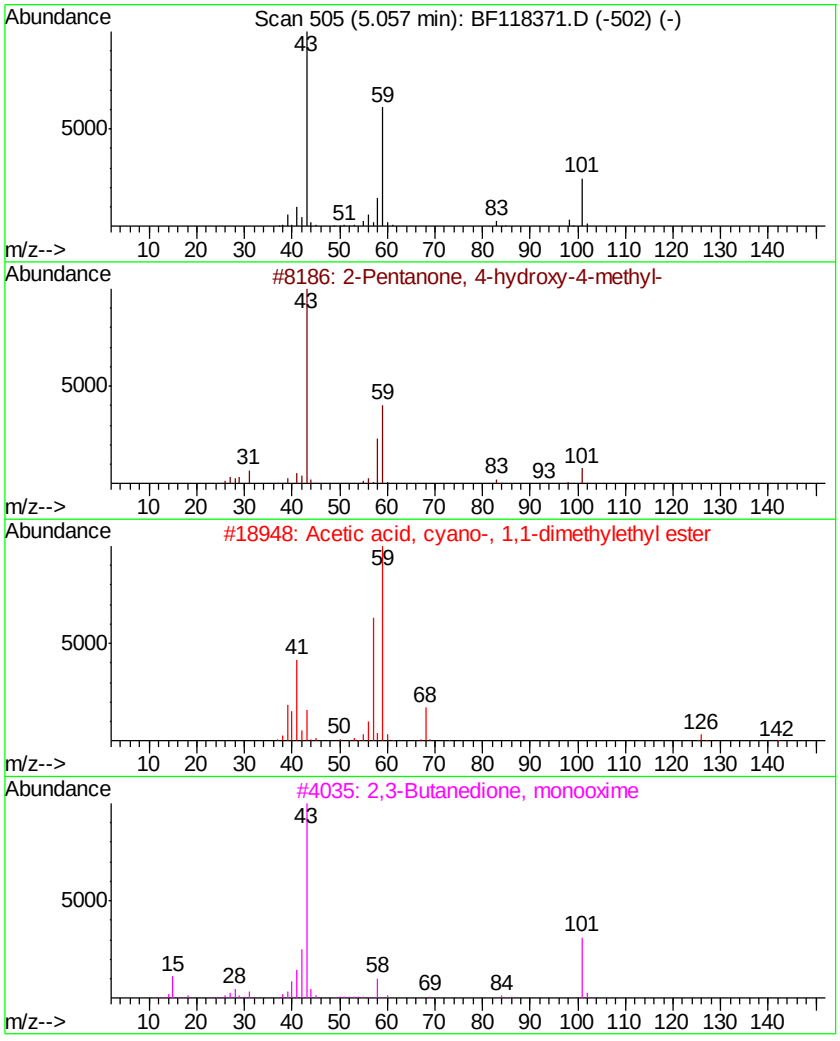
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

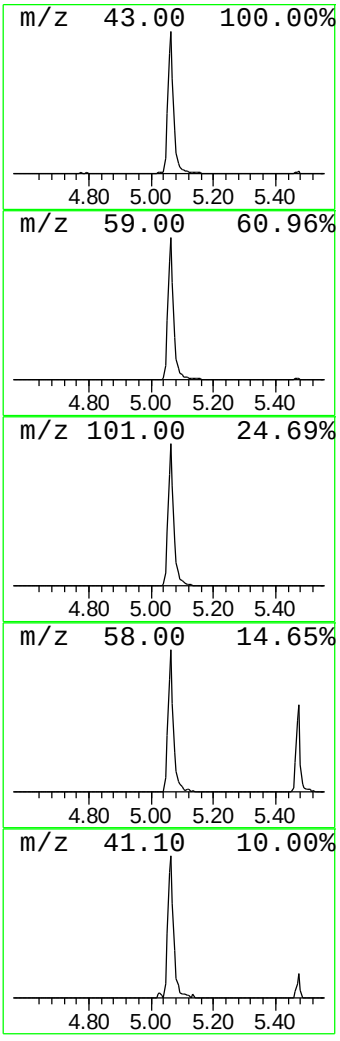
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	18.72 ng	600746	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Acetone	58	C3H6O	000067-64-1	10
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

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Operator : JU
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Misc :
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Instrument : BNA_F
ClientSampleId : DUNR-BF001-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

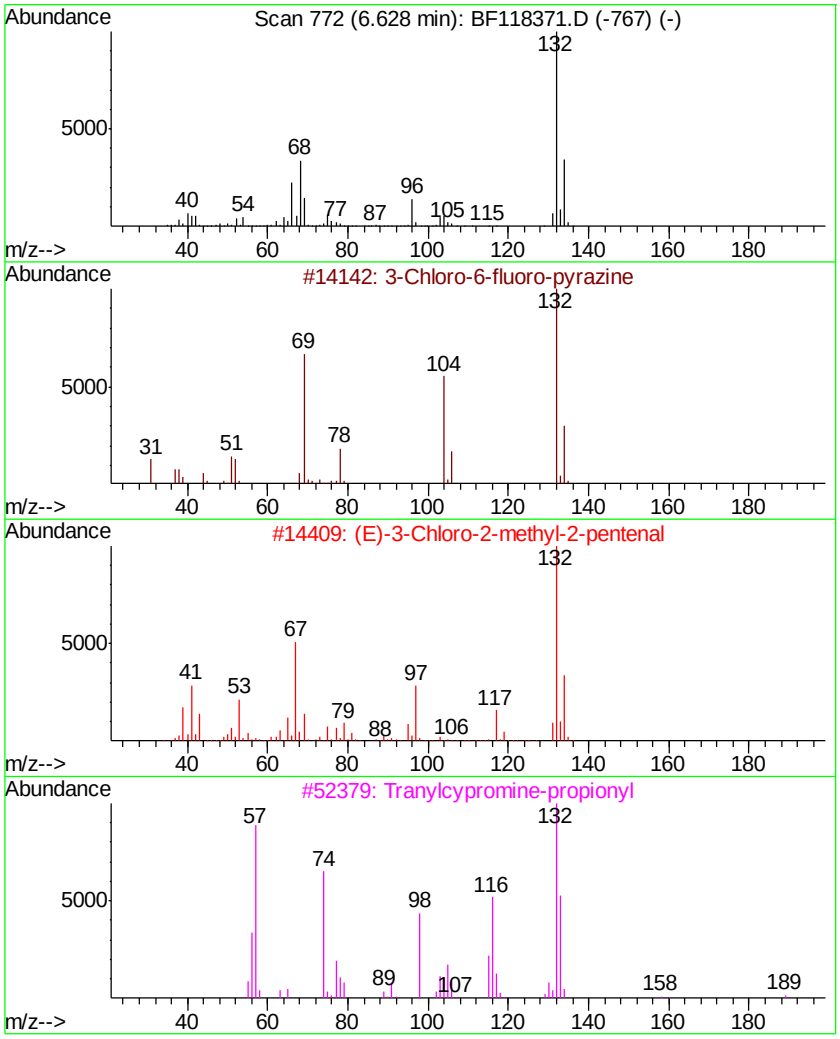
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

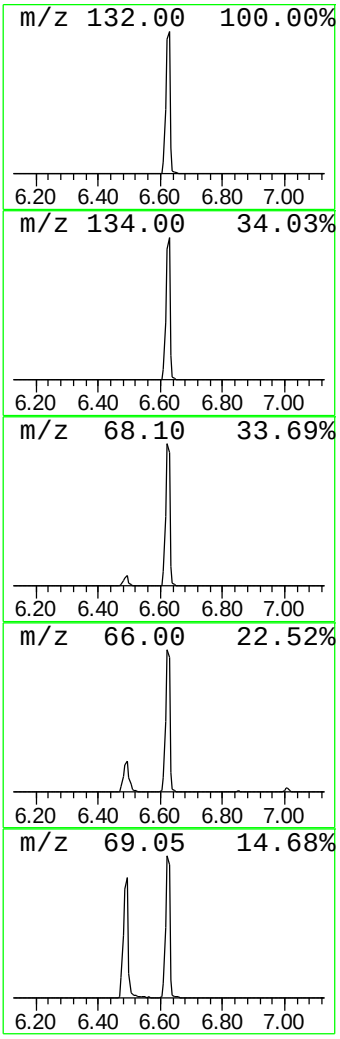
****

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	103.99 ng	3336300	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Instrument : BNA_F
ClientSampleId : DUNR-BF001-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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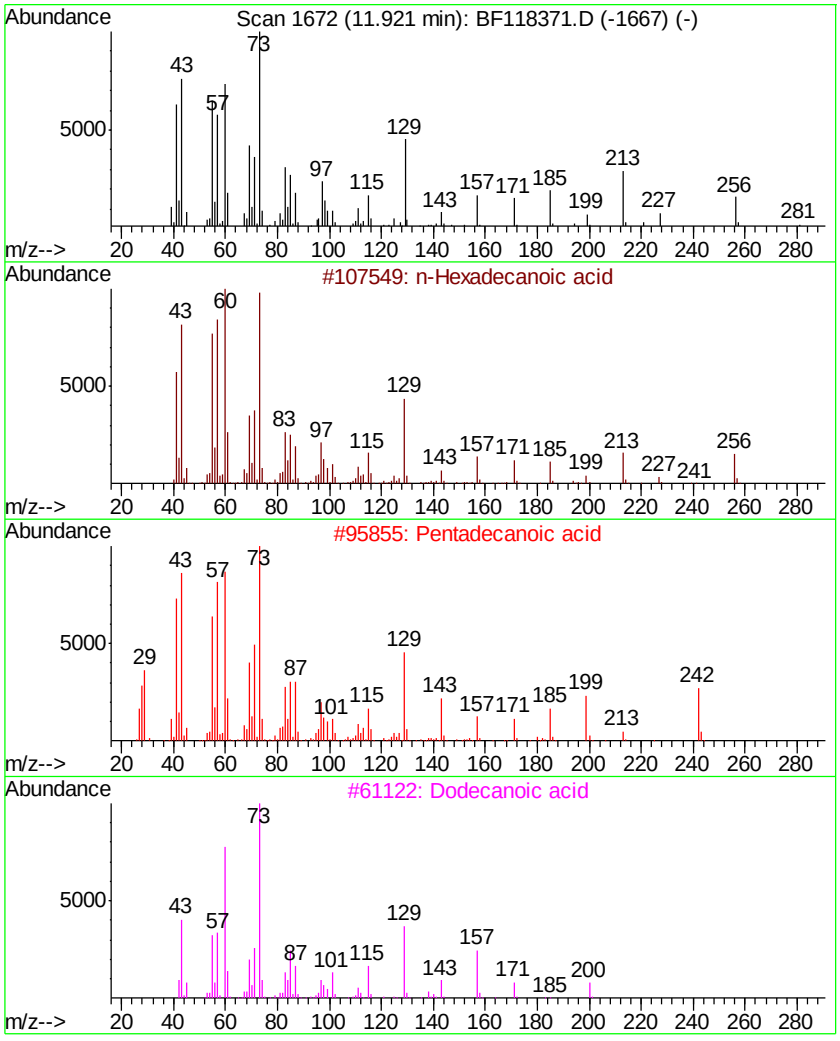
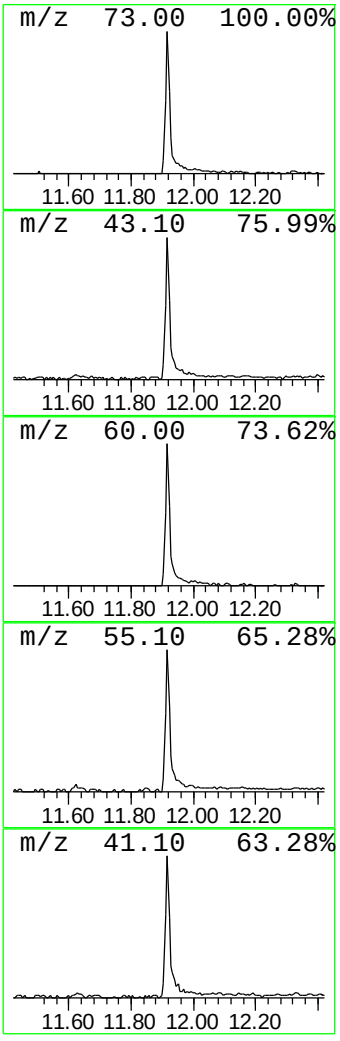
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	7.59 ng	404628	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Dodecanoic acid	200	C12H24O2	000143-07-7	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	70
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUNR-BF001-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

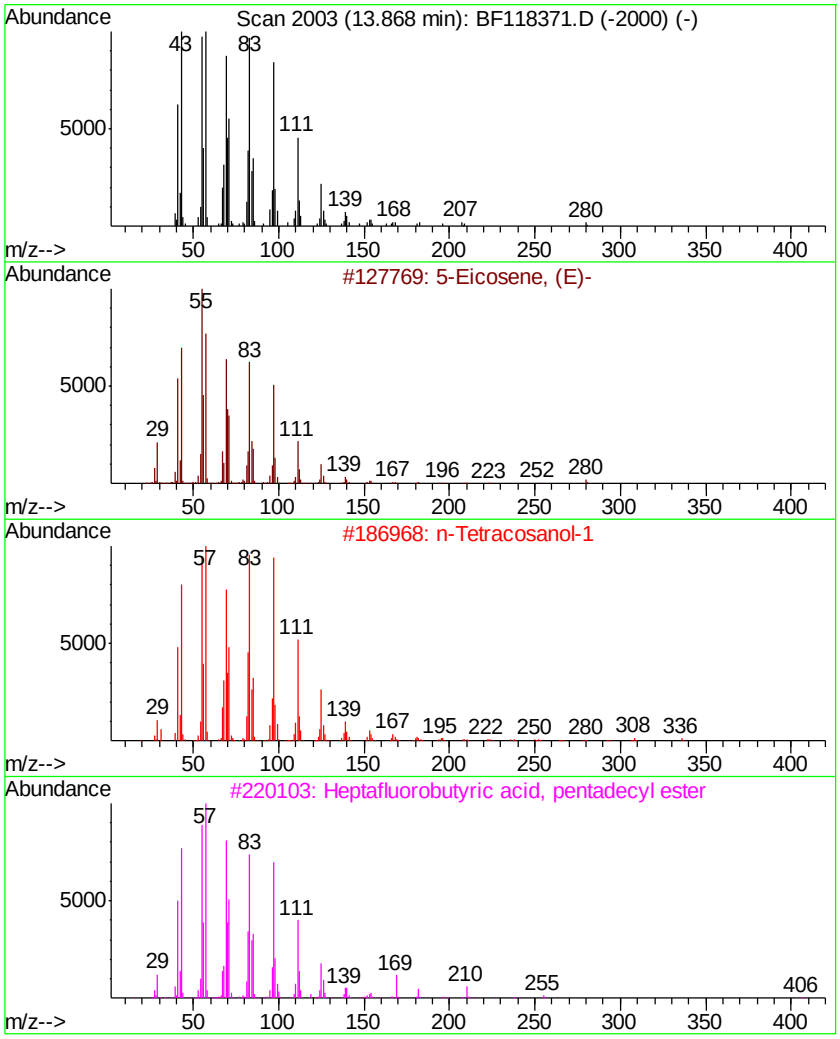
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

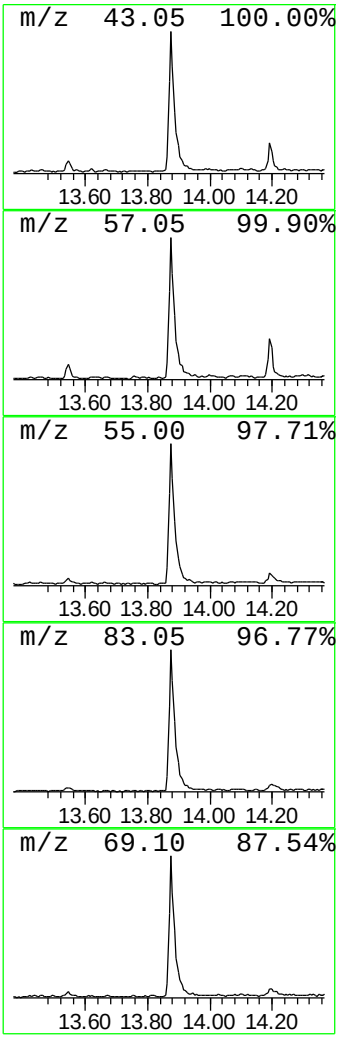
****

Peak Number 5 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	15.18 ng	773611	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





Data Path : Z:\svoasrv\HPCHEM1\BNA F\Data\BF122819\
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Instrument : BNA_F
ClientSampleId : DUNR-BF001-01

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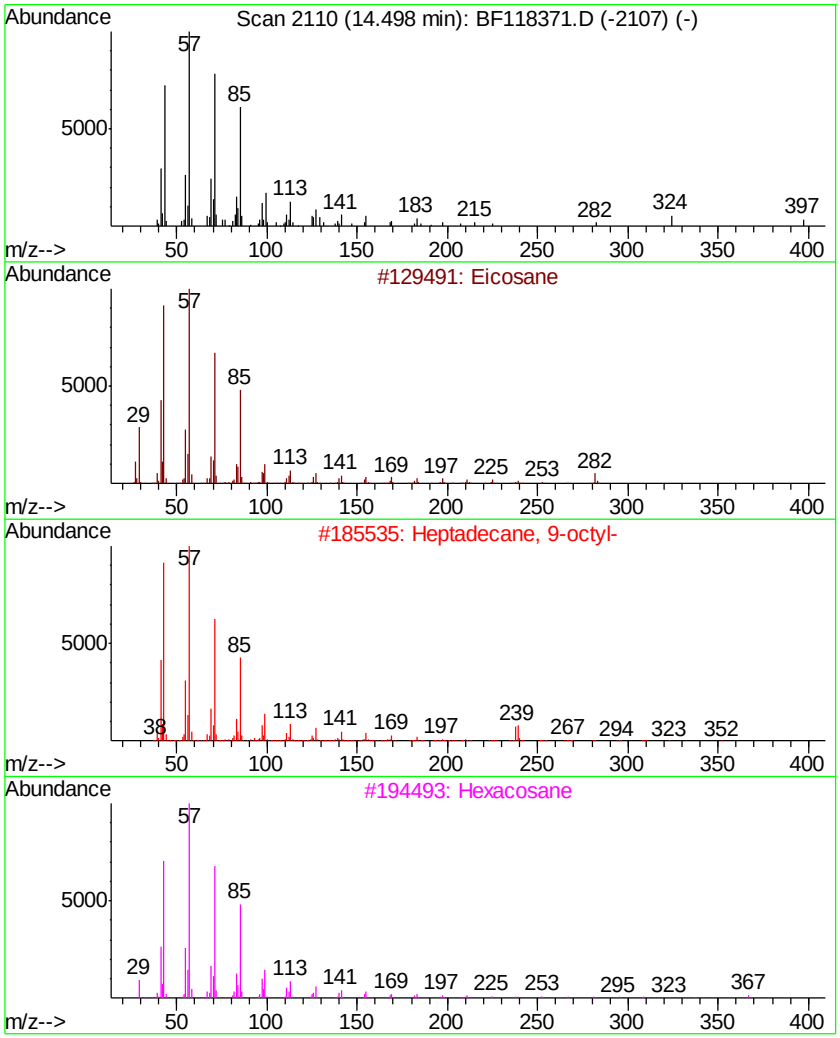
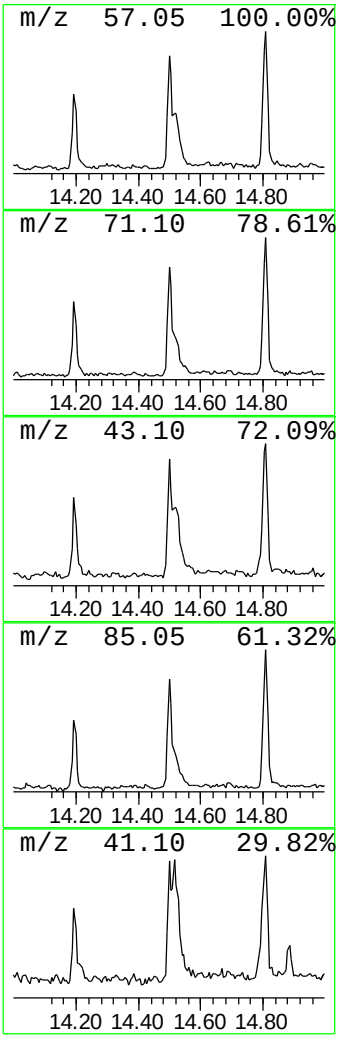
****

Peak Number 6 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	2.61 ng	133145	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87
5	2-methyloctacosane	408	C29H60	1000376-72-8	87





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : DUNR-BF001-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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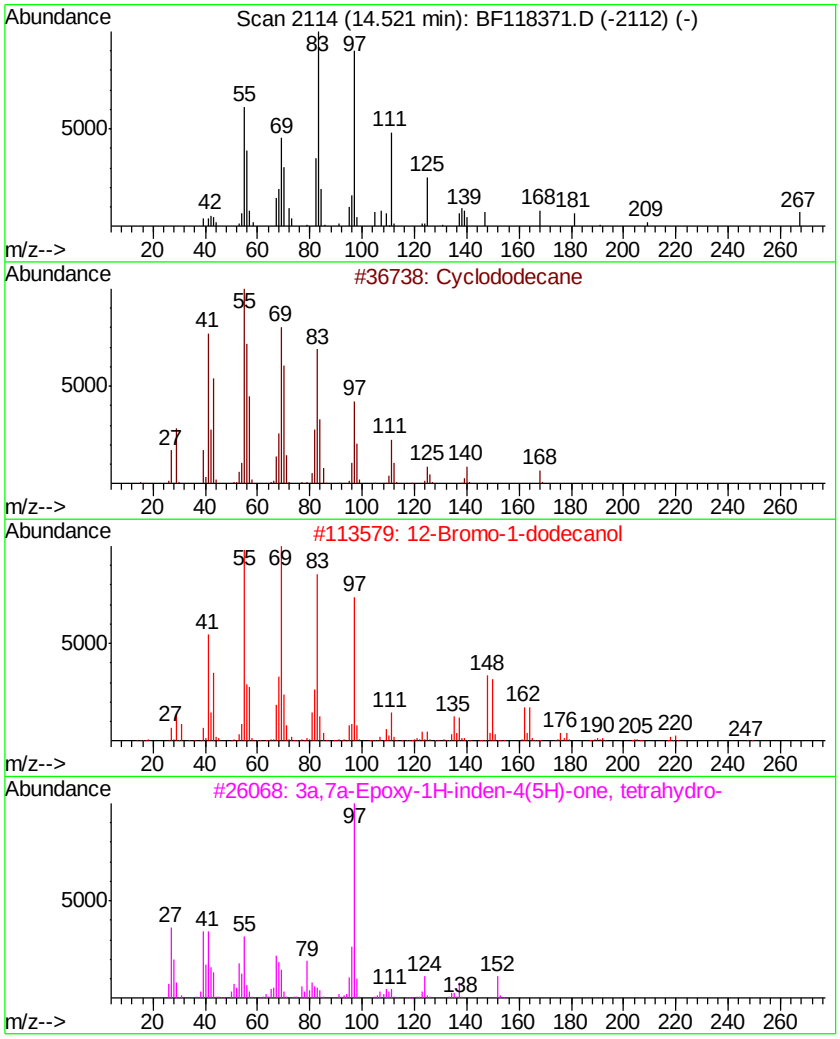
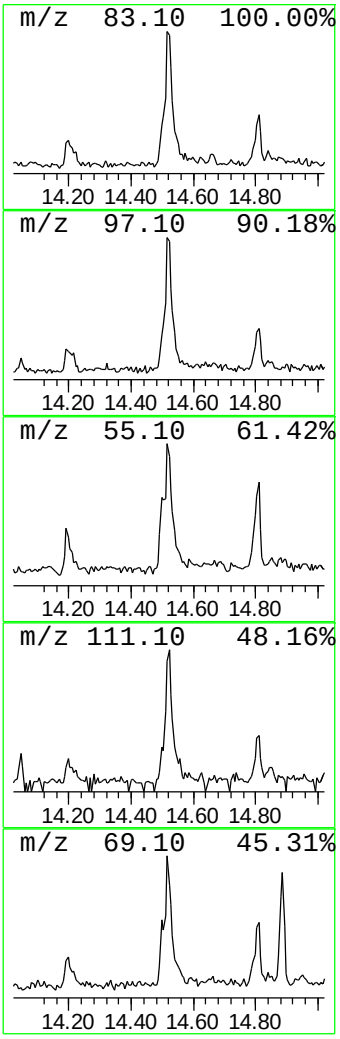
****

Peak Number 7 unknown14.52 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	3.27 ng	166495	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclododecane	168	C12H24	000294-62-2	38
2	12-Bromo-1-dodecanol	264	C12H25BrO	003344-77-2	38
3	3a,7a-Epoxy-1H-inden-4(5H)-one, ...	152	C9H12O2	039746-31-1	30
4	Cyclopentane, pentyl-	140	C10H20	003741-00-2	30
5	Cycloheptane, methyl-	112	C8H16	004126-78-7	27





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Instrument : BNA_F
ClientSampleId : DUNR-BF001-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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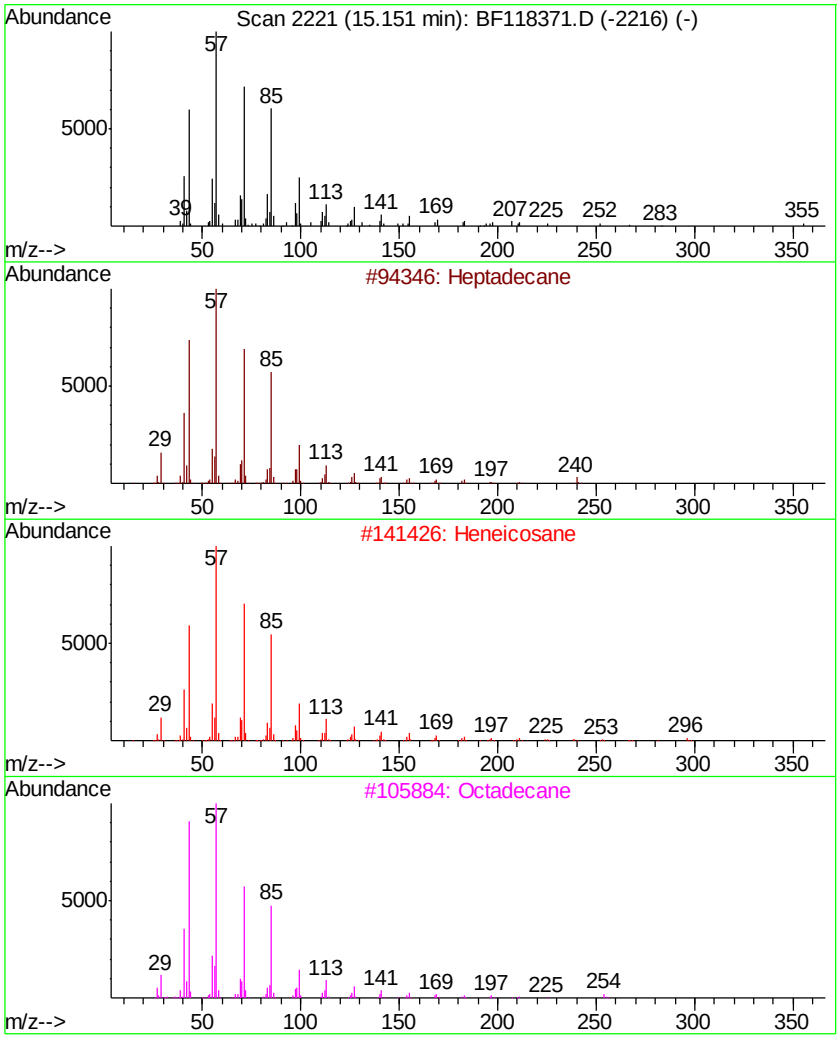
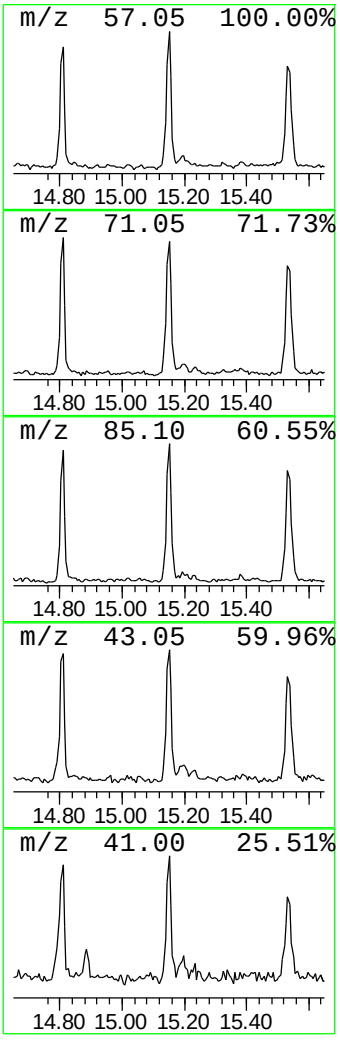
Peak Number 9 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.15	3.12 ng	165367	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octadecane	254	C18H38	000593-45-3	90
4	Tetracosane	338	C24H50	000646-31-1	87
5	Hexacosane	366	C26H54	000630-01-3	87





Library Search Compound Report

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
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TIC Library : C:\DATABASE\NIST11.L
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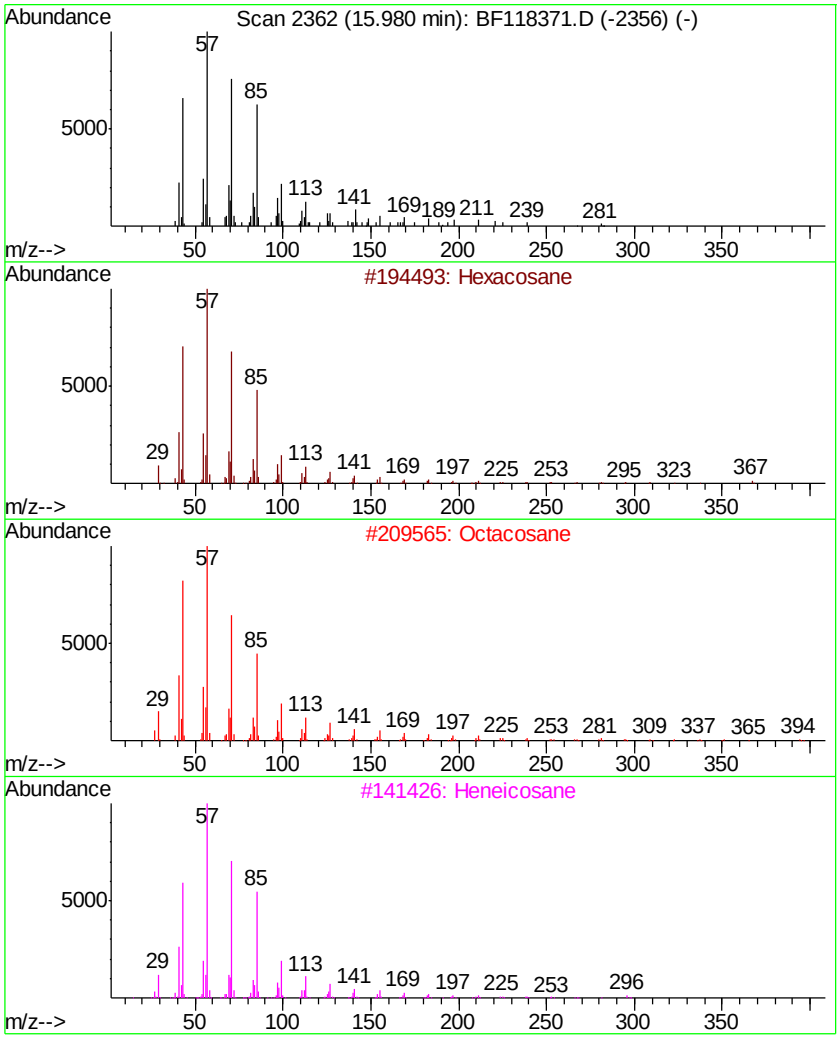
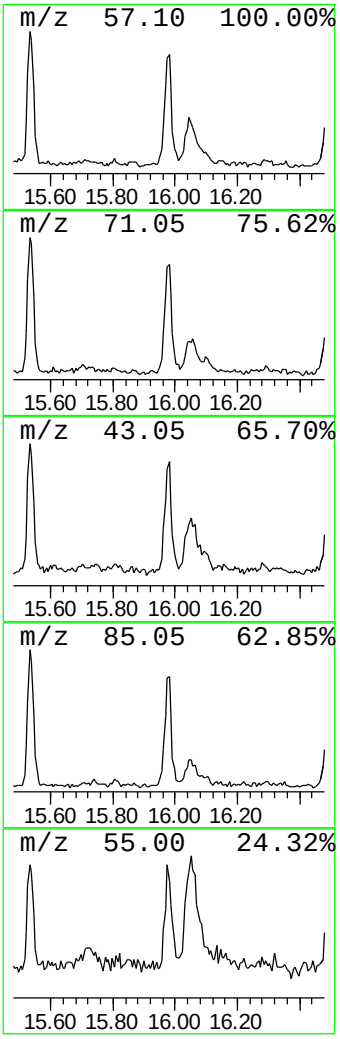
Peak Number 10 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.98	3.03 ng	160535	Perylene-d12	15.54

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





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Acq On : 28 Dec 2019 18:01
Operator : JU
Sample : K6438-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUNR-BF001-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

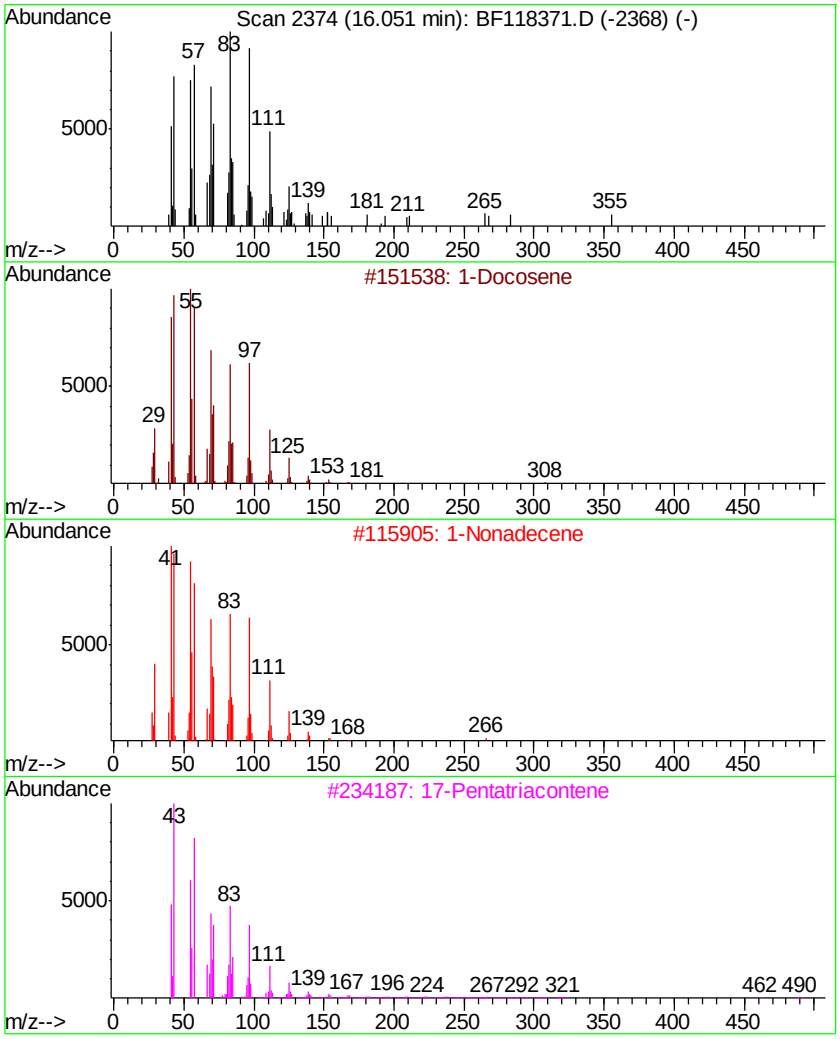
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

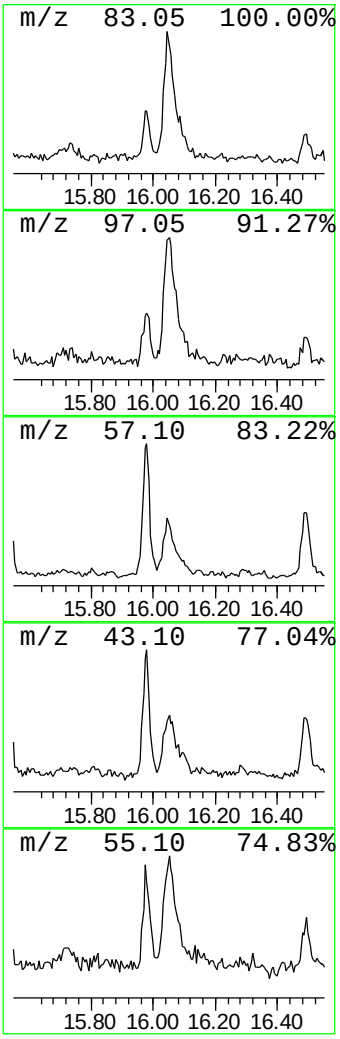
****

Peak Number 11 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.05	3.77 ng	199967	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	91
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	17-Pentatriacontene	491	C35H70	006971-40-0	90
4	10-Heneicosene (c,t)	294	C21H42	095008-11-0	90
5	Heptacosyl acetate	438	C29H58O2	1000351-78-2	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122819\
Data File : BF118371.D
Acq On : 28 Dec 2019 18:01
Operator : JU
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Misc :
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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
2-Pentanone, 4-hy...	5.06	18.7	ng	600746	1	6.85	641666	20.0
unknown6.63	6.63	104.0	ng	3336300	1	6.85	641666	20.0
n-Hexadecanoic acid	11.92	7.6	ng	404628	4	11.39	1065740	20.0
5-Eicosene, (E)-	13.87	15.2	ng	773611	5	14.04	1019160	20.0
Eicosane	14.50	2.6	ng	133145	5	14.04	1019160	20.0
unknown14.52	14.52	3.3	ng	166495	5	14.04	1019160	20.0
Heptadecane	15.15	3.1	ng	165367	6	15.54	1060480	20.0
Hexacosane	15.98	3.0	ng	160535	6	15.54	1060480	20.0
1-Docosene	16.05	3.8	ng	199967	6	15.54	1060480	20.0