LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070919\
Data File : BF115441.D
Acq On : 9 Jul 2019 19:01
Operator : HP/JU
Sample : K3687-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STONES

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-BF070519.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	2.216	14	22	29	rBV	1164525	1574604	39.79%	4.803%
2	5.516	578	583	586	rBV	2749320	2492943	62.99%	7.605%
3	6.516	747	753	756	rBV	2740171	2667998	67.42%	8.139%
4	6.663	773	778	781	rBV	3099582	2783317	70.33%	8.490%
5	6.892	814	817	821	rVB	1144135	936812	23.67%	2.858%
6	7.051	840	844	847	rBV	2671884	2251213	56.89%	6.867%
7	7.451	907	912	915	rBV	1907782	1724519	43.58%	5.261%
8	8.175	1031	1035	1038	rBV	1488797	1198483	30.28%	3.656%
9	9.251	1213	1218	1221	rBV	3857370	3424745	86.54%	10.447%
10	9.639	1280	1284	1294	rBV	192659	171024	4.32%	0.522%
11	9.927	1329	1333	1349	rVB	1626078	1466233	37.05%	4.473%
12	10.710	1462	1466	1481	rBV	1846595	1951200	49.30%	5.952%
13	11.410	1581	1585	1589	rBV	1842771	1561979	39.47%	4.765%
14	13.015	1853	1858	1861	rBV	4010998	3957437	100.00%	12.072%
15	14.010	2022	2027	2043	rBV2	110500	295833	7.48%	0.902%
16	14.157	2048	2052	2059	rVV	1316780	1290749	32.62%	3.937%
17	14.368	2084	2088	2093	rBV	67533	72033	1.82%	0.220%
18	14.739	2146	2151	2155	rBV	133847	150581	3.81%	0.459%
19	15.098	2208	2212	2218	rBV	235324	257679	6.51%	0.786%
20	15.468	2270	2275	2280	rBV	307967	368281	9.31%	1.123%
21	15.786	2323	2329	2338	rBV	786979	1028417	25.99%	3.137%
22	15.868	2338	2343	2352	rVV	334696	432769	10.94%	1.320%
23	16.327	2415	2421	2430	rBV	258177	402124	10.16%	1.227%
24	16.856	2505	2511	2519	rVB	125298	232486	5.87%	0.709%
25	17.474	2610	2616	2624	rVB2	42743	88740	2.24%	0.271%

Sum of corrected areas: 32782199

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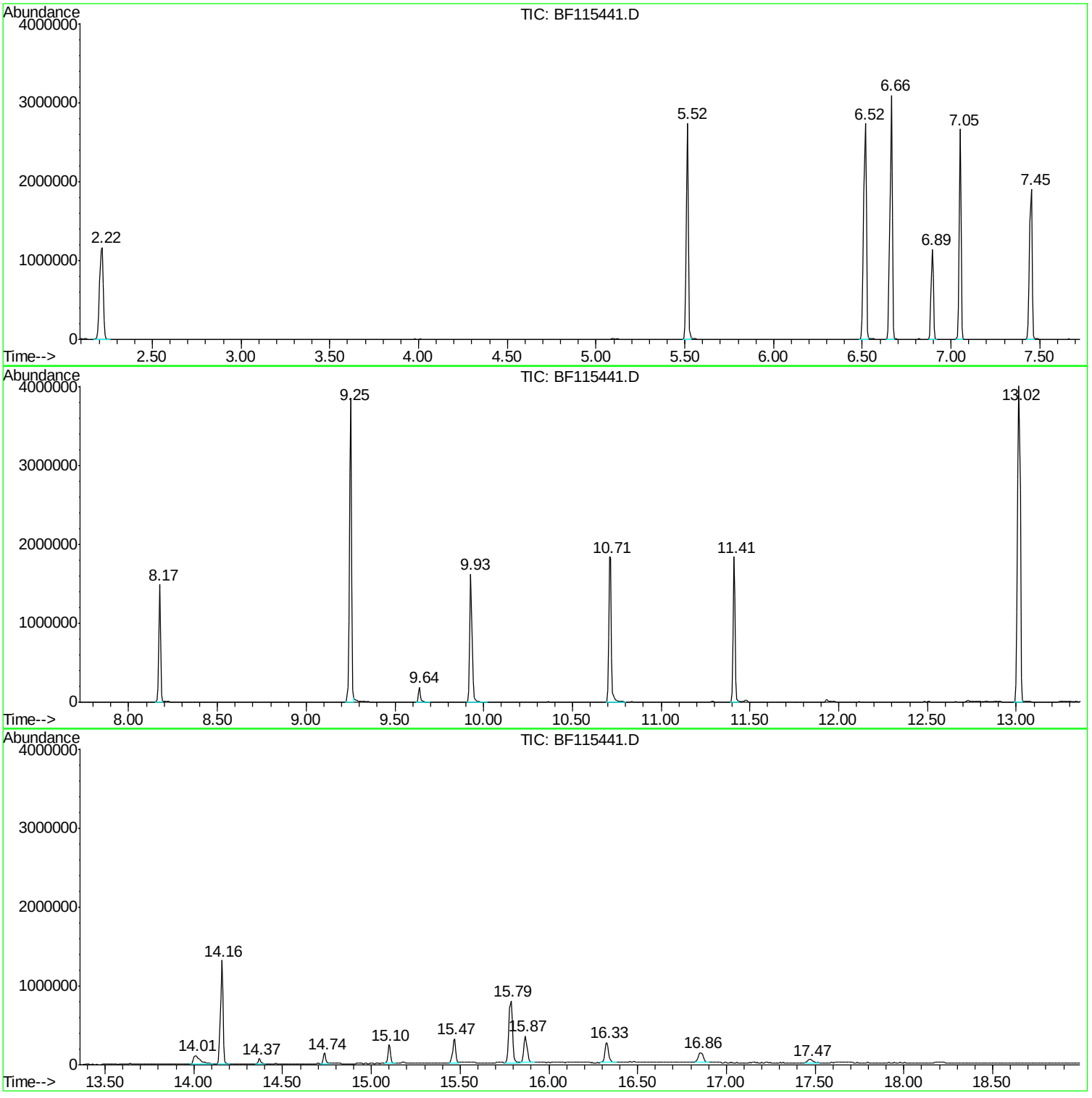
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STONES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.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\BF070919\
Data File : BF115441.D
Acq On : 9 Jul 2019 19:01
Operator : HP/JU
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Misc :
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Instrument : BNA_F
ClientSampleId : STONES

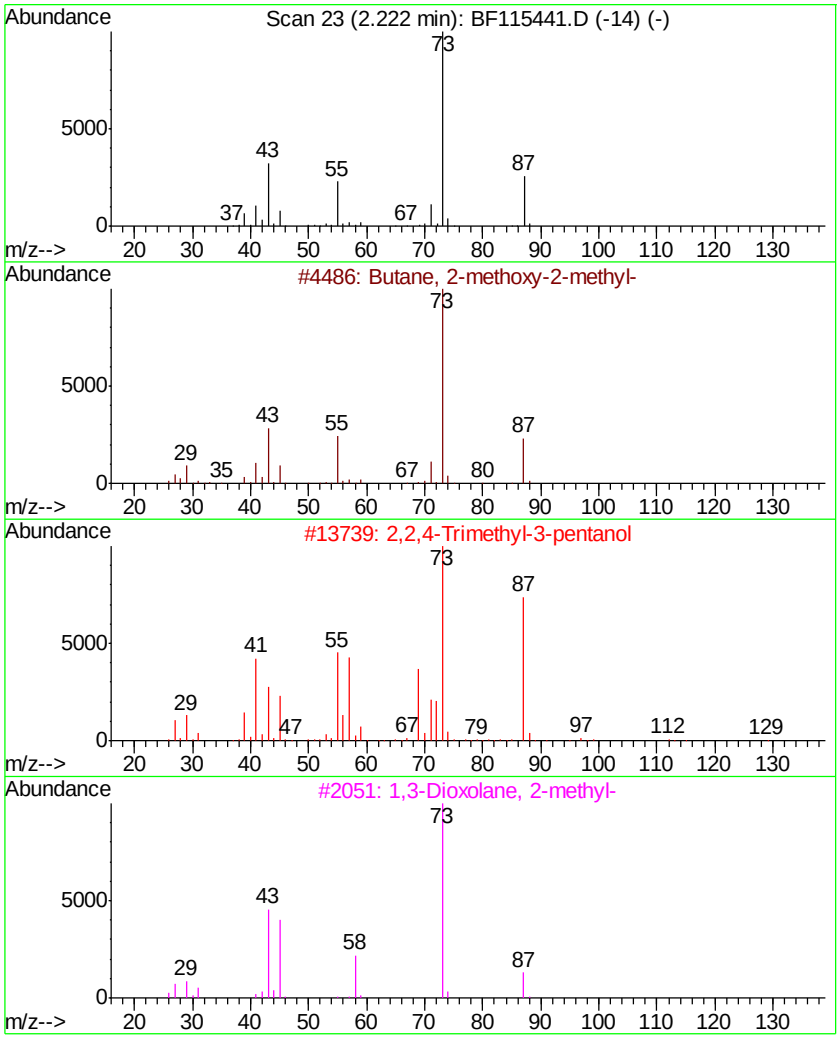
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

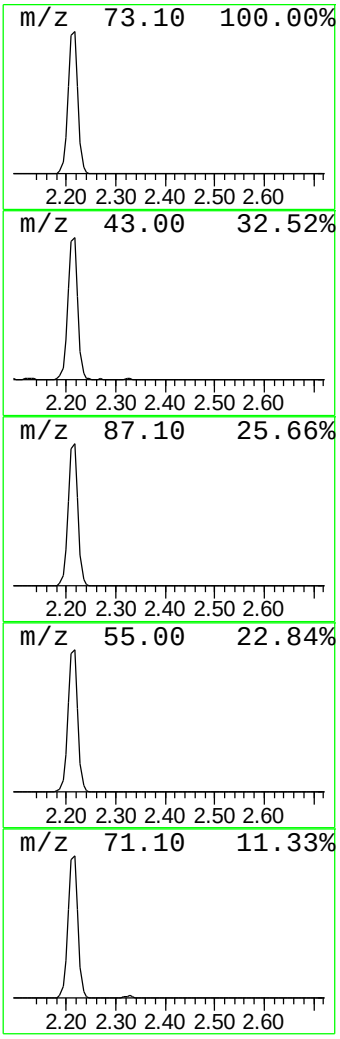
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	33.62 ng	1574600	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	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





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Data File : BF115441.D
Acq On : 9 Jul 2019 19:01
Operator : HP/JU
Sample : K3687-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STONES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

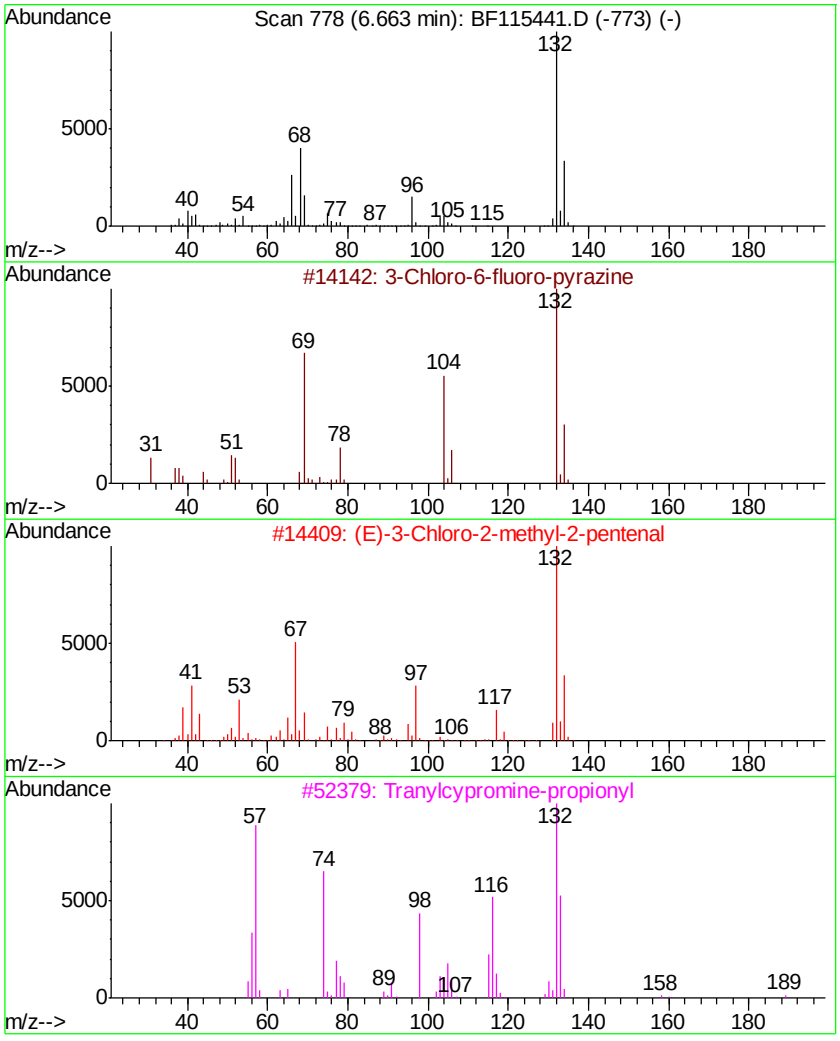
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

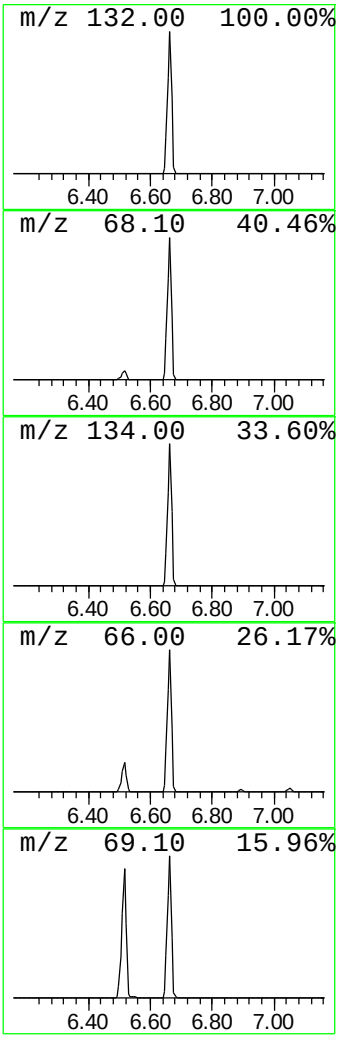
****

Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	59.42 ng	2783320	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	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Xenon	132	Xe	007440-63-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070919\
Data File : BF115441.D
Acq On : 9 Jul 2019 19:01
Operator : HP/JU
Sample : K3687-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STONES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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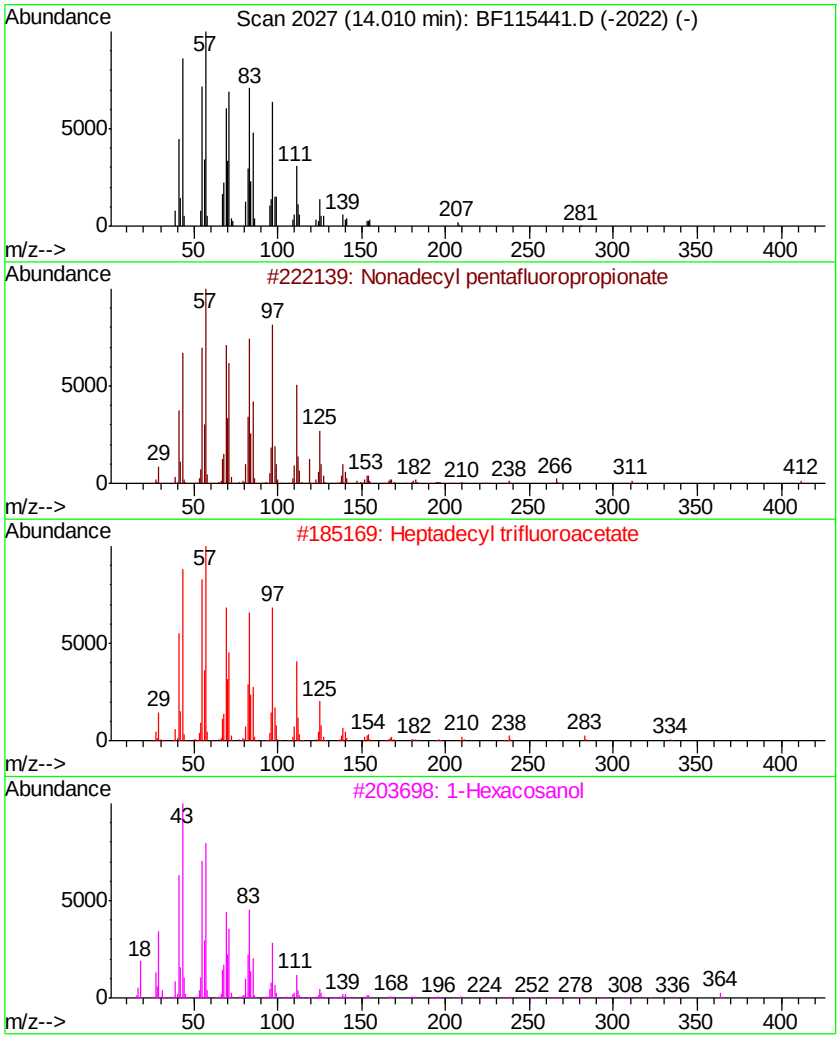
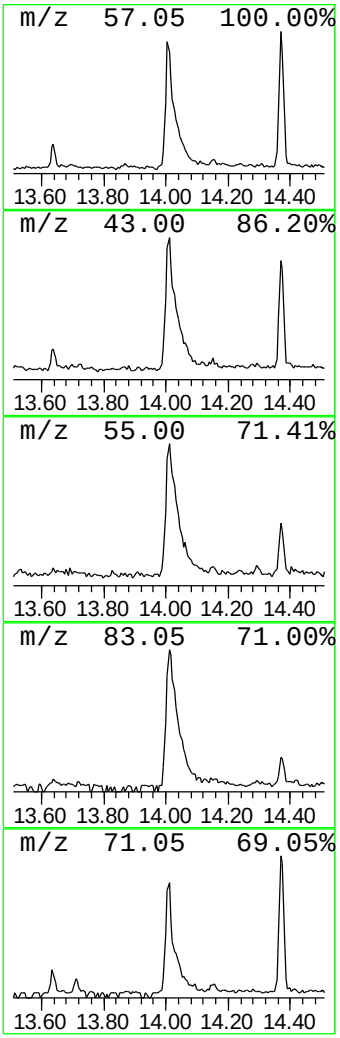
Peak Number 4 Nonadecyl pentafluoropropio... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.01	4.58 ng	295833	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	90
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	87
3	1-Hexacosanol	382	C26H54O	000506-52-5	83
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	83
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	81





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070919\
Data File : BF115441.D
Acq On : 9 Jul 2019 19:01
Operator : HP/JU
Sample : K3687-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STONES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.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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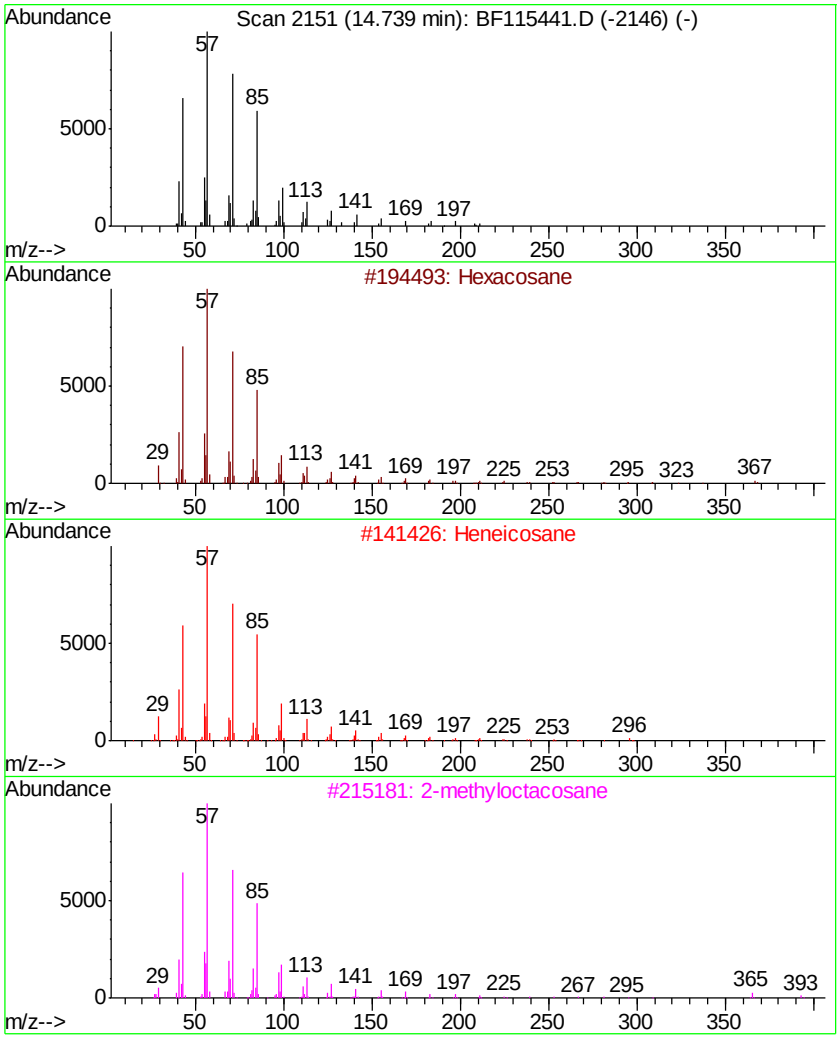
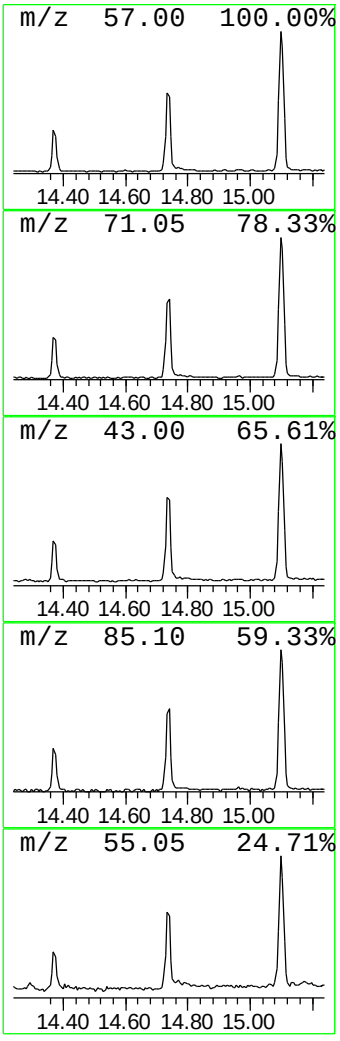
Peak Number 5 Docosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.74	2.33 ng	150581	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Triacontane	422	C30H62	000638-68-6	90
5	Docosane	310	C22H46	000629-97-0	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070919\
Data File : BF115441.D
Acq On : 9 Jul 2019 19:01
Operator : HP/JU
Sample : K3687-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STONES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.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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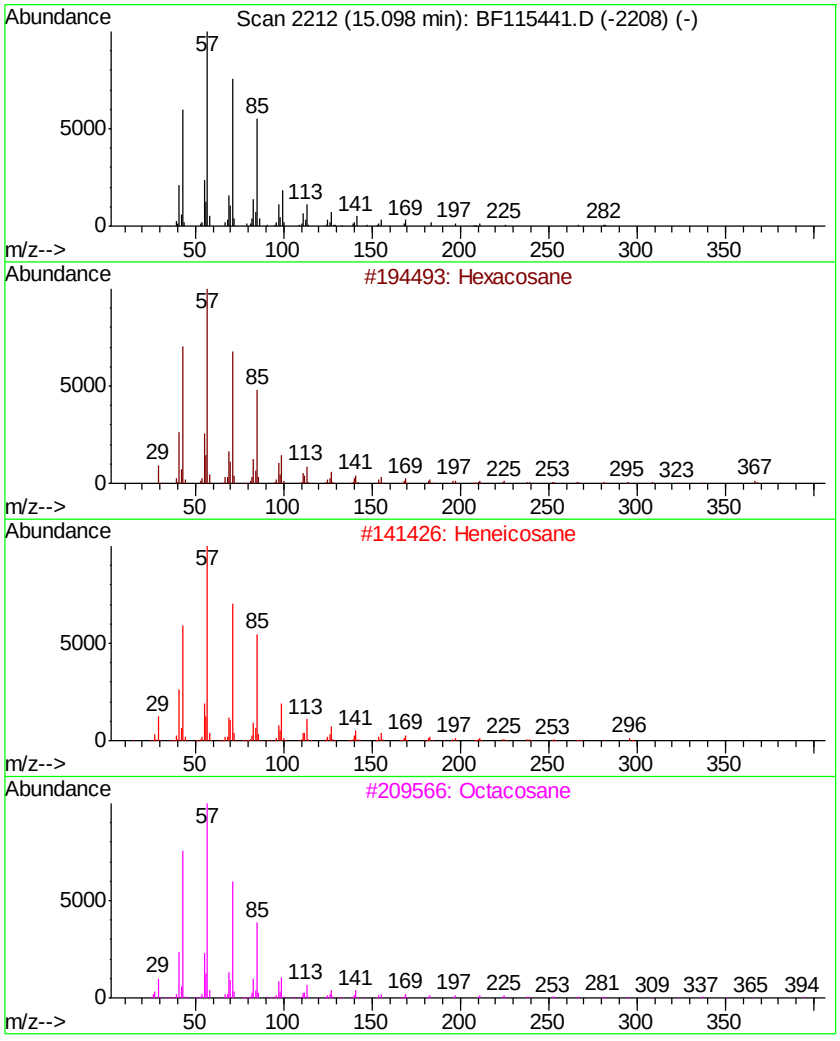
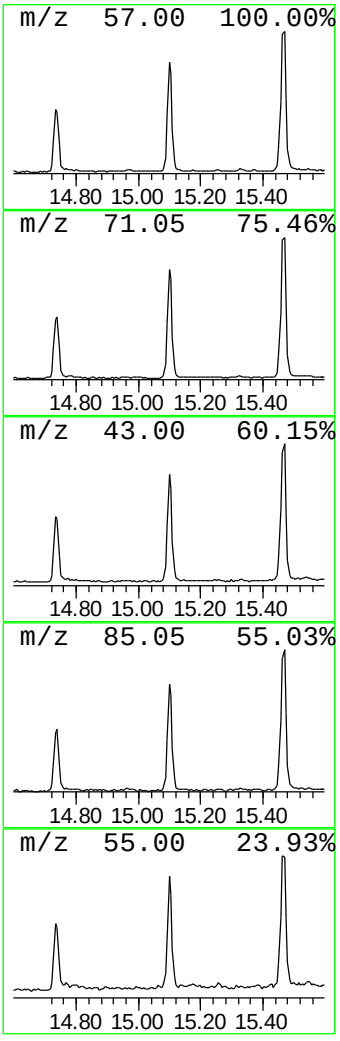
Peak Number 6 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.10	5.01 ng	257679	Perylene-d12	15.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane	394	C28H58	000630-02-4	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Octadecane	254	C18H38	000593-45-3	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070919\
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Acq On : 9 Jul 2019 19:01
Operator : HP/JU
Sample : K3687-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STONES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.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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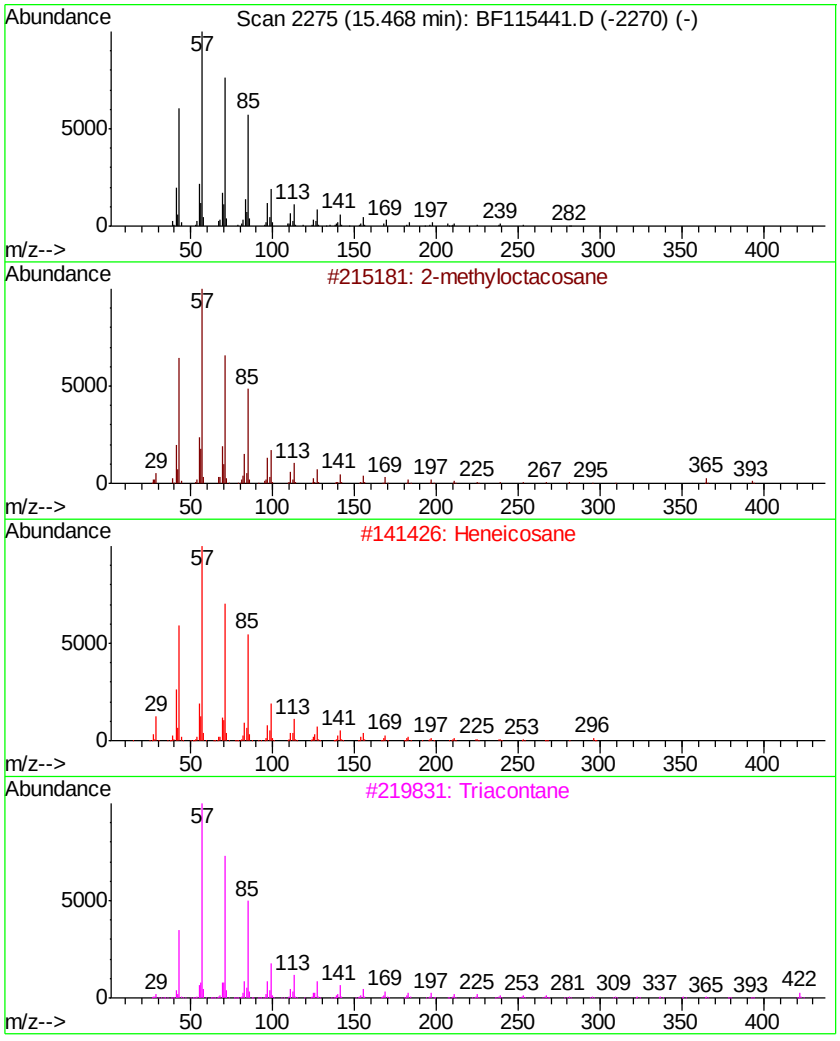
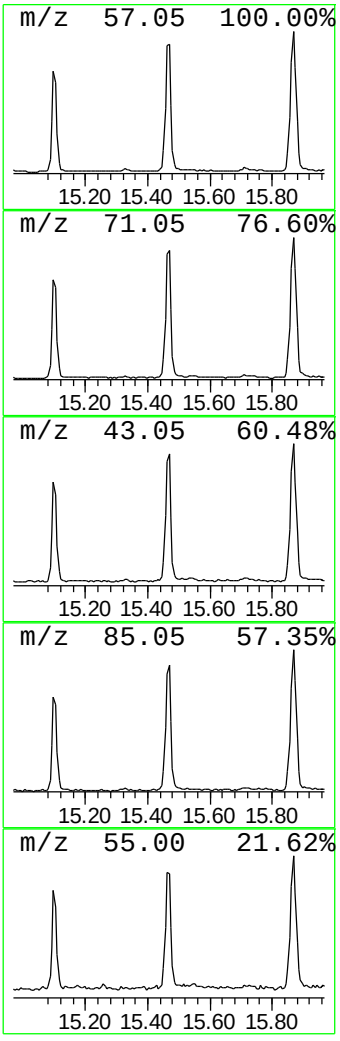
Peak Number 7 2-methyloctacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.47	7.16 ng	368281	Perylene-d12	15.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	91





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ClientSampleId : STONES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.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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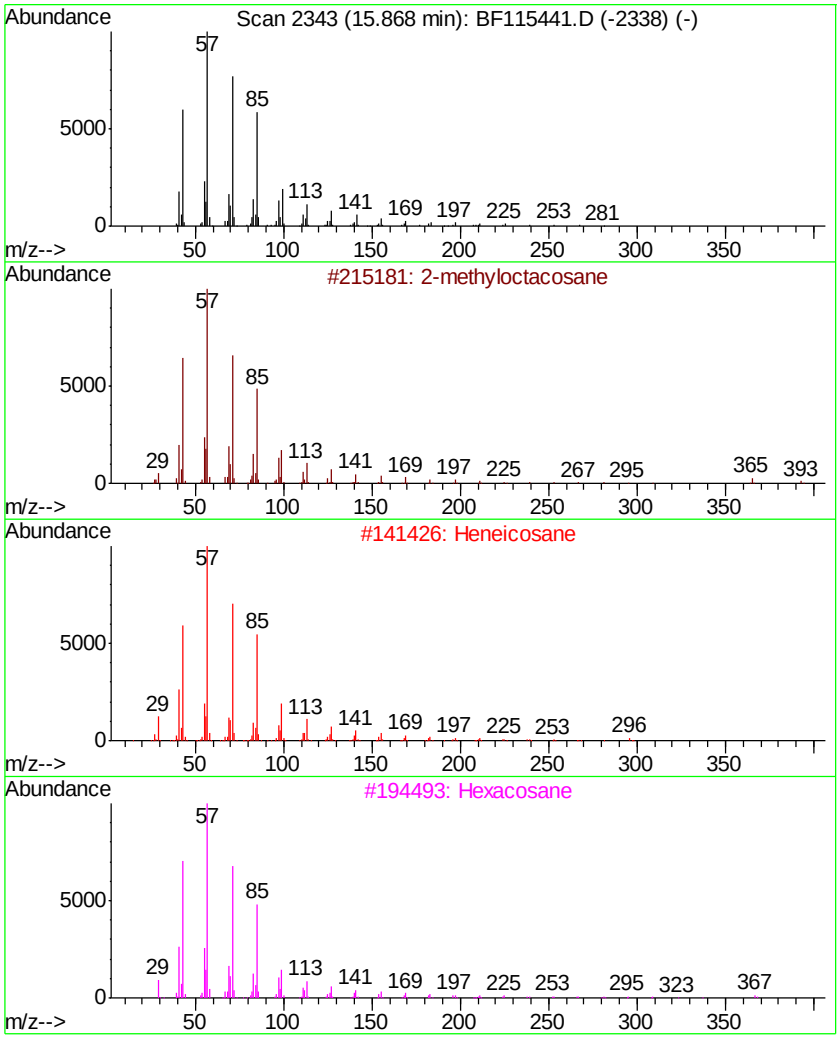
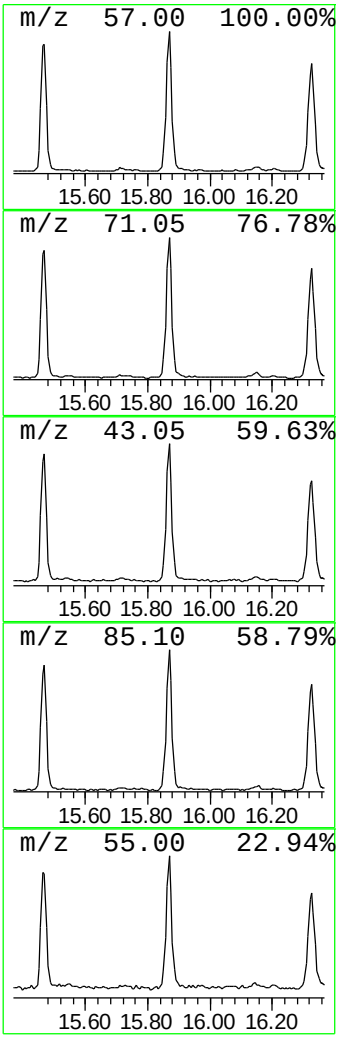
Peak Number 8 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	8.42 ng	432769	Perylene-d12	15.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Heptadecane	240	C17H36	000629-78-7	91





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Misc :
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Instrument : BNA_F
ClientSampleId : STONES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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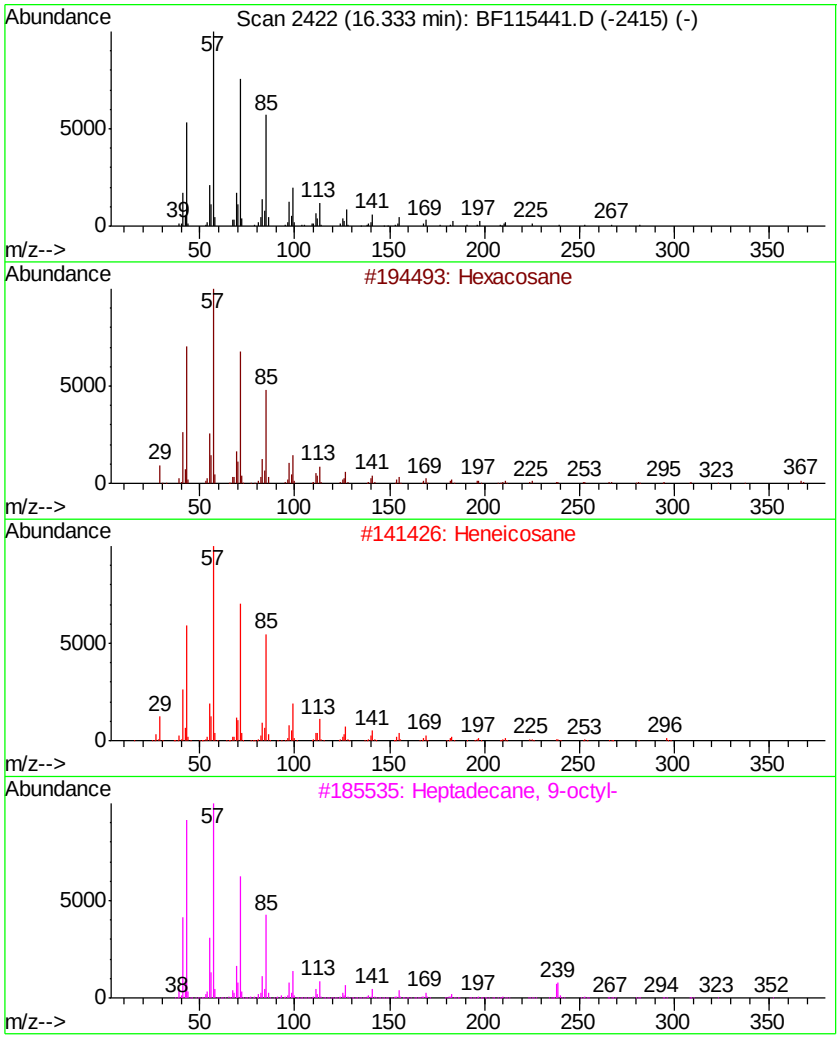
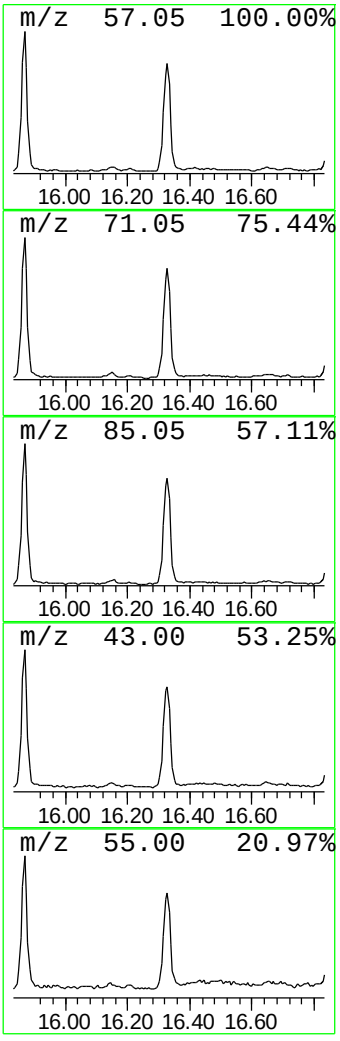
Peak Number 9 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.33	7.82 ng	402124	Perylene-d12	15.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Heptadecane	240	C17H36	000629-78-7	91





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Instrument : BNA_F
ClientSampleId : STONES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.M
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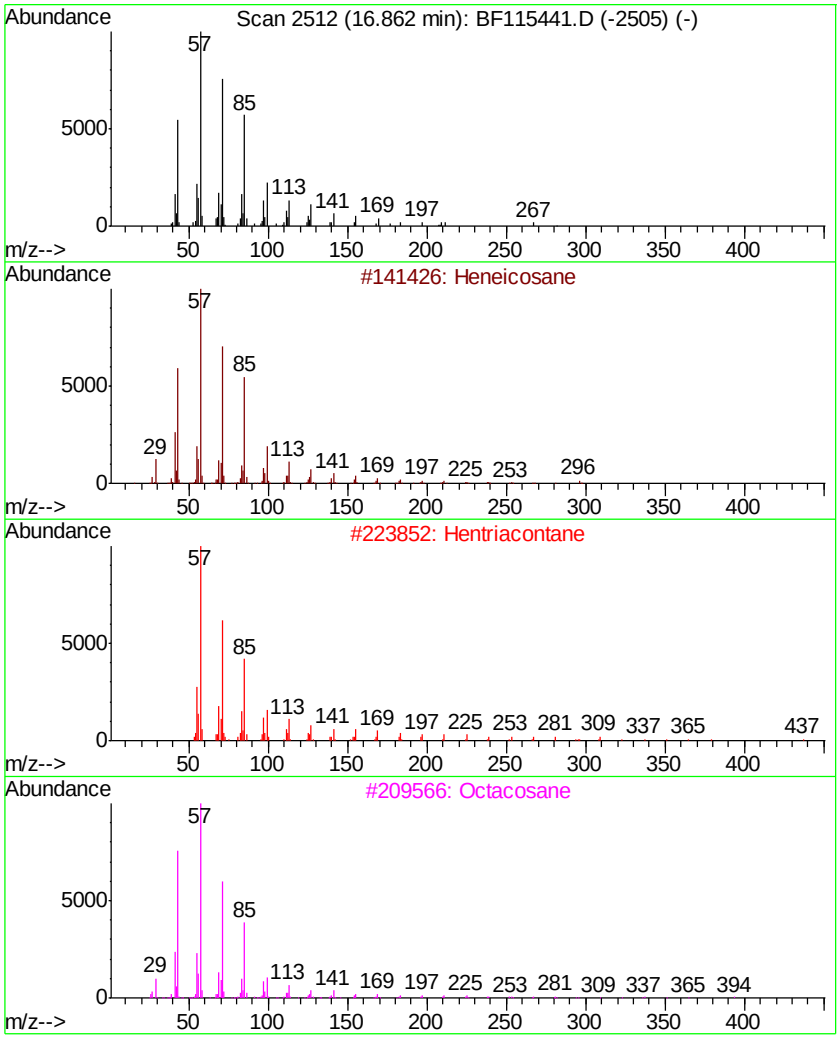
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

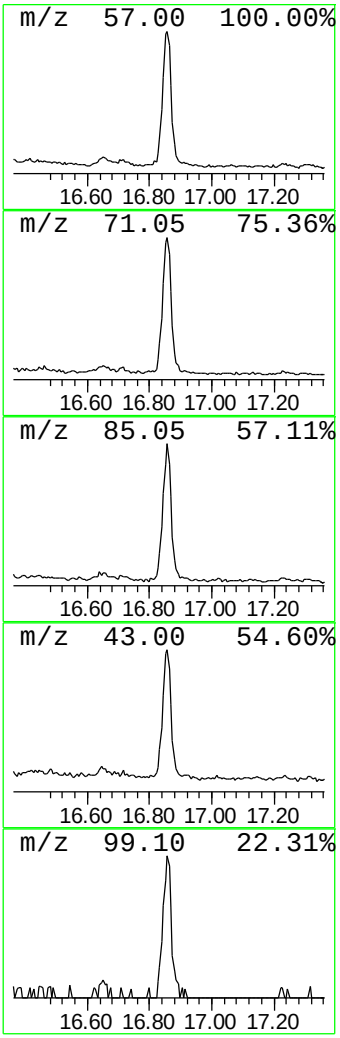
****

Peak Number 10 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.86	4.52 ng	232486	Perylene-d12	15.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hentriacontane	437	C31H64	000630-04-6	91
3	Octacosane	394	C28H58	000630-02-4	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Hexacosane	366	C26H54	000630-01-3	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF070919\
Data File : BF115441.D
Acq On : 9 Jul 2019 19:01
Operator : HP/JU
Sample : K3687-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STONES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.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...	2.22	33.6	ng	1574600	1	6.89	936812	20.0
unknown6.66	6.66	59.4	ng	2783320	1	6.89	936812	20.0
Nonadecyl pentafl...	14.01	4.6	ng	295833	5	14.16	1290750	20.0
Docosane	14.74	2.3	ng	150581	5	14.16	1290750	20.0
Heneicosane	15.10	5.0	ng	257679	6	15.79	1028420	20.0
2-methyloctacosane	15.47	7.2	ng	368281	6	15.79	1028420	20.0
Heptacosane	15.87	8.4	ng	432769	6	15.79	1028420	20.0
Hexacosane	16.33	7.8	ng	402124	6	15.79	1028420	20.0
Octacosane	16.86	4.5	ng	232486	6	15.79	1028420	20.0