LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040319\
Data File : BF113554.D
Acq On : 3 Apr 2019 20:16
Operator : JU/SJ
Sample : K2213-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S9A-S9B-S9C

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-BF040319.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	5.298	542	546	564	rBV	2562213	2607869	96.83%	10.019%
2	6.334	718	722	739	rBV	2696469	2693326	100.00%	10.347%
3	6.457	739	743	746	rBV	3049603	2671342	99.18%	10.262%
4	6.686	778	782	792	rBV	756502	684083	25.40%	2.628%
5	6.839	804	808	824	rBV	2344188	2105841	78.19%	8.090%
6	7.251	873	878	892	rBV	1665696	1653729	61.40%	6.353%
7	7.963	996	999	1015	rBV	816689	805690	29.91%	3.095%
8	9.045	1179	1183	1186	rBV	3208193	2664681	98.94%	10.237%
9	9.439	1247	1250	1255	rBV	145765	128437	4.77%	0.493%
10	9.722	1294	1298	1310	rVB	860488	792458	29.42%	3.044%
11	10.510	1428	1432	1450	rBV	1694289	1590669	59.06%	6.111%
12	11.204	1546	1550	1553	rBV	883169	752828	27.95%	2.892%
13	11.745	1638	1642	1644	rBV2	27570	34667	1.29%	0.133%
14	12.416	1752	1756	1759	rBV	168010	147331	5.47%	0.566%
15	12.527	1770	1775	1780	rBV5	37376	66372	2.46%	0.255%
16	12.604	1785	1788	1790	rBV	39634	34294	1.27%	0.132%
17	12.639	1790	1794	1797	rVB	149495	145376	5.40%	0.558%
18	12.786	1815	1819	1822	rBV	2667578	2428303	90.16%	9.329%
19	12.815	1822	1824	1828	rVB2	61887	51370	1.91%	0.197%
20	12.974	1844	1851	1853	rVB4	18223	35325	1.31%	0.136%
21	13.027	1856	1860	1864	rBV2	61488	71509	2.66%	0.275%
22	13.368	1914	1918	1921	rVB	64003	61715	2.29%	0.237%
23	13.692	1971	1973	1976	rBV	77000	86094	3.20%	0.331%
24	13.721	1976	1978	1990	rVB5	44251	113882	4.23%	0.437%
25	13.839	1993	1998	2001	rBV	922816	977015	36.28%	3.753%
26	14.010	2023	2027	2031	rBV	107570	111514	4.14%	0.428%
27	14.315	2075	2079	2082	rVB	138371	138182	5.13%	0.531%
28	14.609	2125	2129	2132	rBV	196706	204461	7.59%	0.785%
29	14.851	2167	2170	2177	rBV	119971	210755	7.83%	0.810%
30	14.921	2178	2182	2186	rVB	208047	231787	8.61%	0.890%
31	15.133	2215	2218	2224	rVB	64578	75946	2.82%	0.292%
32	15.192	2225	2228	2233	rVV	54440	61679	2.29%	0.237%
33	15.251	2233	2238	2247	rVB2	593712	997002	37.02%	3.830%
34	15.668	2305	2309	2317	rVB	193674	263695	9.79%	1.013%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040319\
Data File : BF113554.D
Acq On : 3 Apr 2019 20:16
Operator : JU/SJ
Sample : K2213-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S9A-S9B-S9C

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-BF040319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.127	2383	2387	2403	rVB	141821	331190	12.30%	1.272%

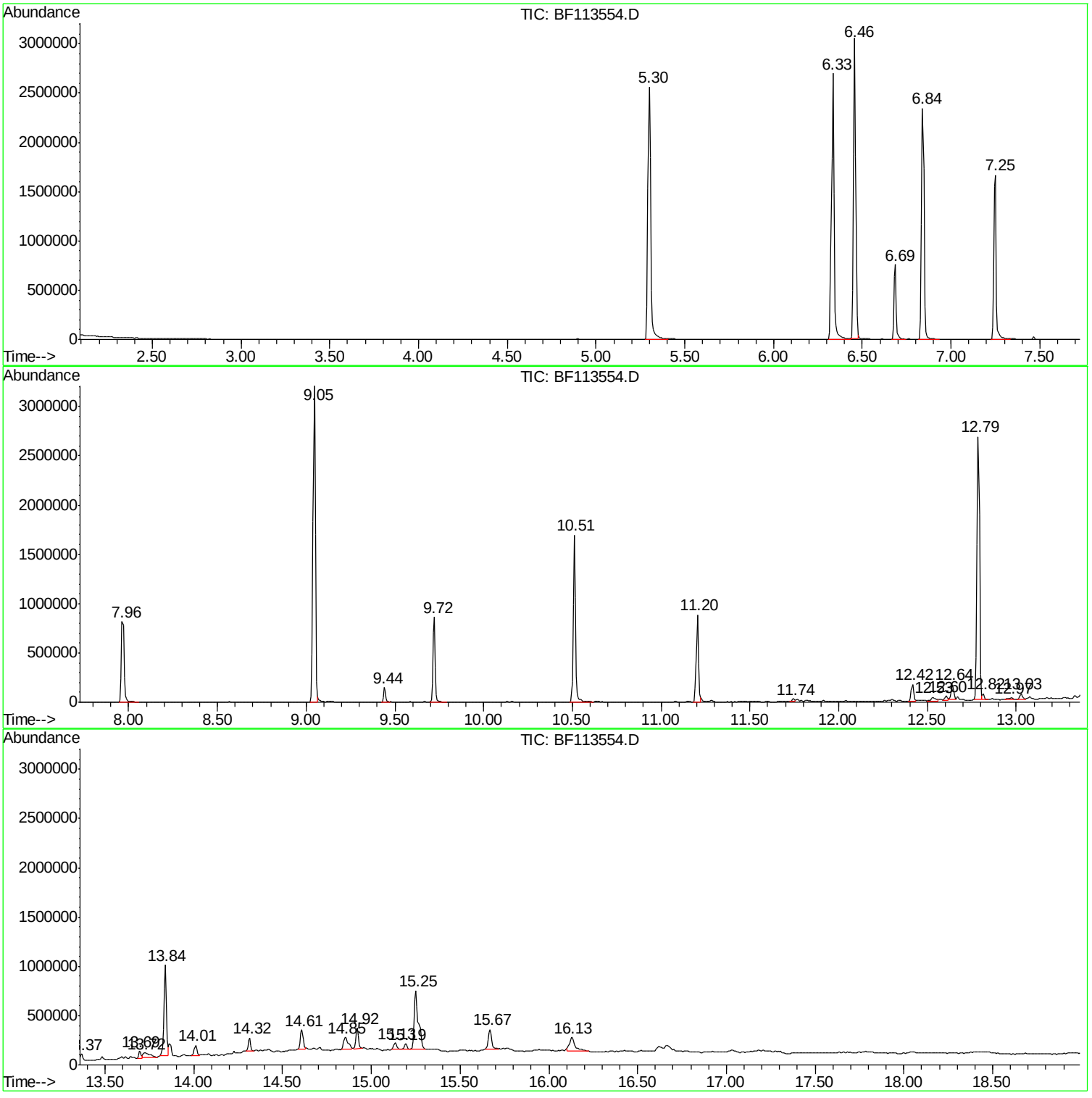
Sum of corrected areas: 26030417

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040319\
Data File : BF113554.D
Acq On : 3 Apr 2019 20:16
Operator : JU/SJ
Sample : K2213-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S9A-S9B-S9C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040319\
Data File : BF113554.D
Acq On : 3 Apr 2019 20:16
Operator : JU/SJ
Sample : K2213-03
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

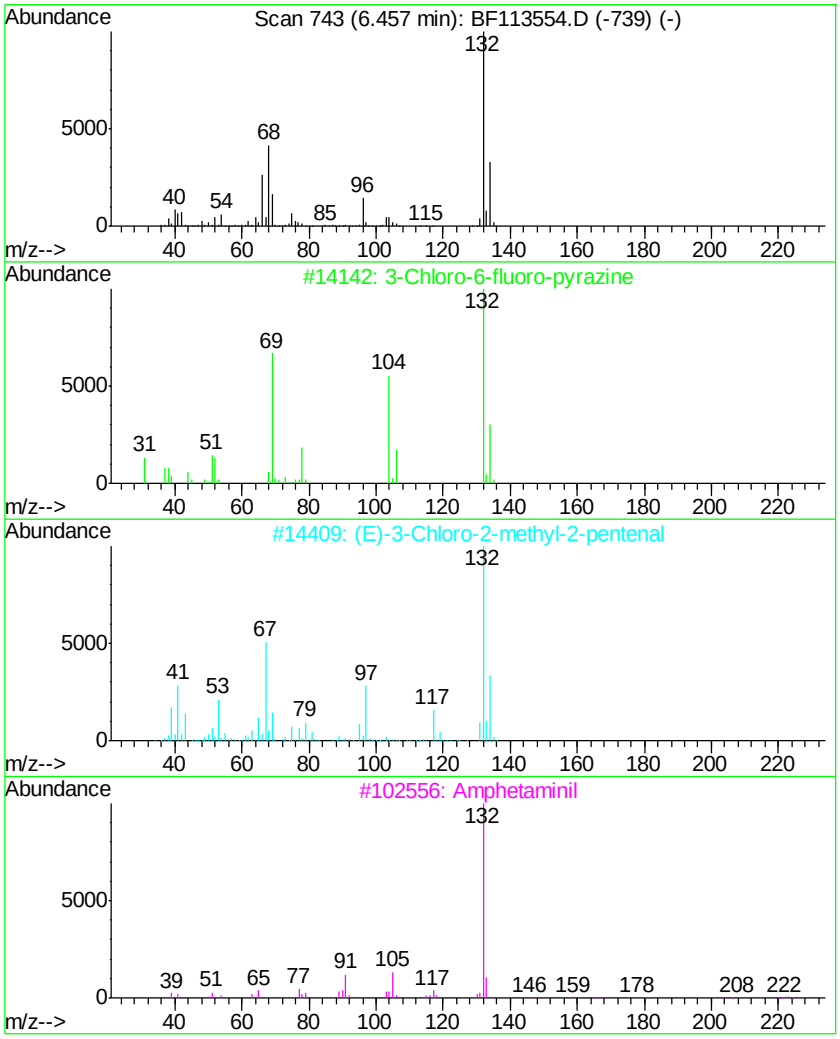
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

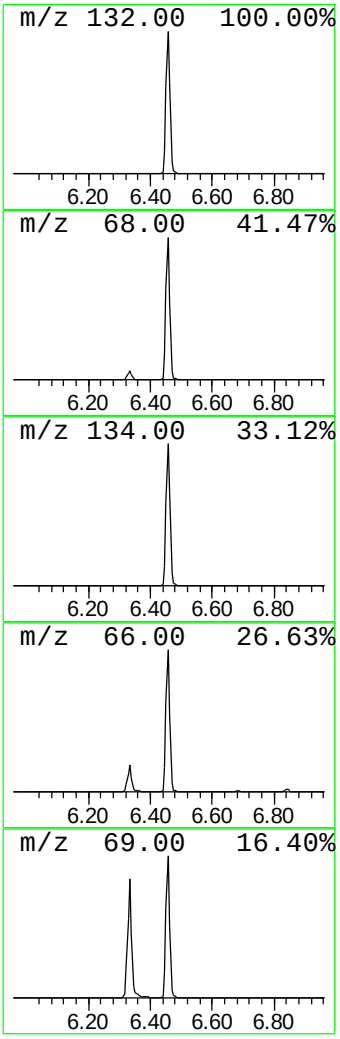
****

Peak Number 1 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	78.10 ng	2671340	1,4-Dichlorobenzene-d4	6.69

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	Amphetaminil	250	C17H18N2	017590-01-1	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	5-Aminoindole	132	C8H8N2	005192-03-0	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040319\
Data File : BF113554.D
Acq On : 3 Apr 2019 20:16
Operator : JU/SJ
Sample : K2213-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S9A-S9B-S9C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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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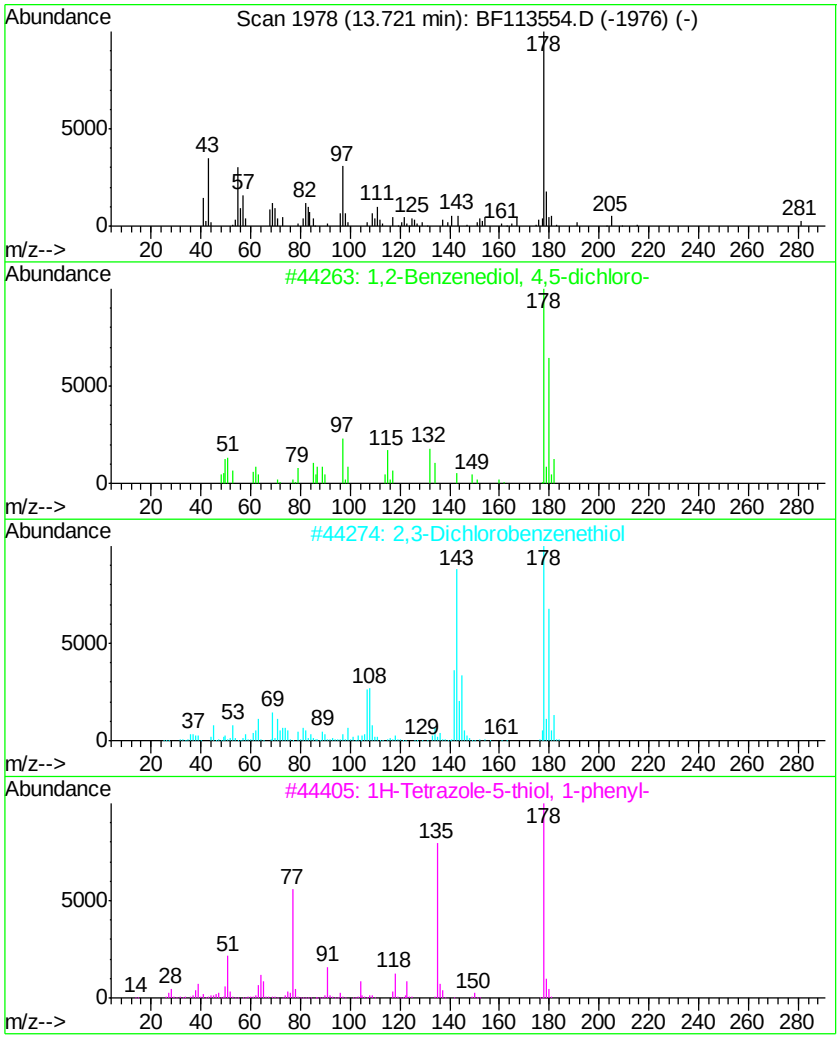
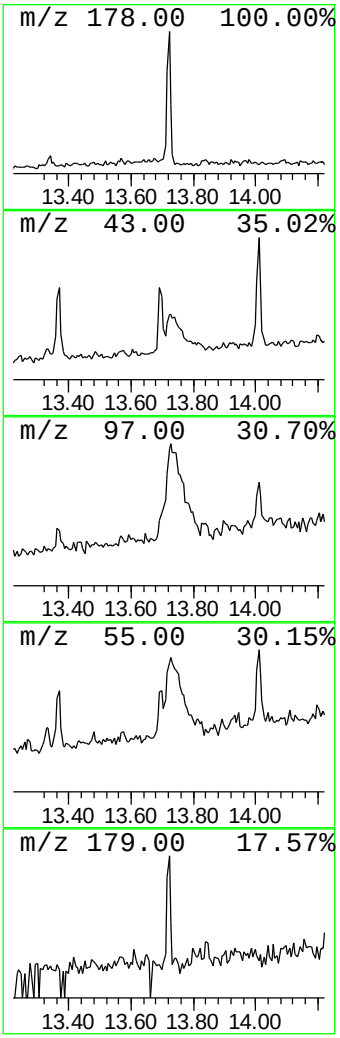
Peak Number 3 1,2-Benzenediol, 4,5-dichloro- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	2.33 ng	113882	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenediol, 4,5-dichloro-	178	C6H4Cl2O2	003428-24-8	59
2	2,3-Dichlorobenzenethiol	178	C6H4Cl2S	017231-95-7	50
3	1H-Tetrazole-5-thiol, 1-phenyl-	178	C7H6N4S	000086-93-1	50
4	2-Propenoic acid, 3-[4-[(3-methy...	246	C15H18O3	055256-10-5	50
5	Iminodiacetic acid, N-[[5-fluore...	355	C19H17NO6	112918-82-8	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040319\
Data File : BF113554.D
Acq On : 3 Apr 2019 20:16
Operator : JU/SJ
Sample : K2213-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S9A-S9B-S9C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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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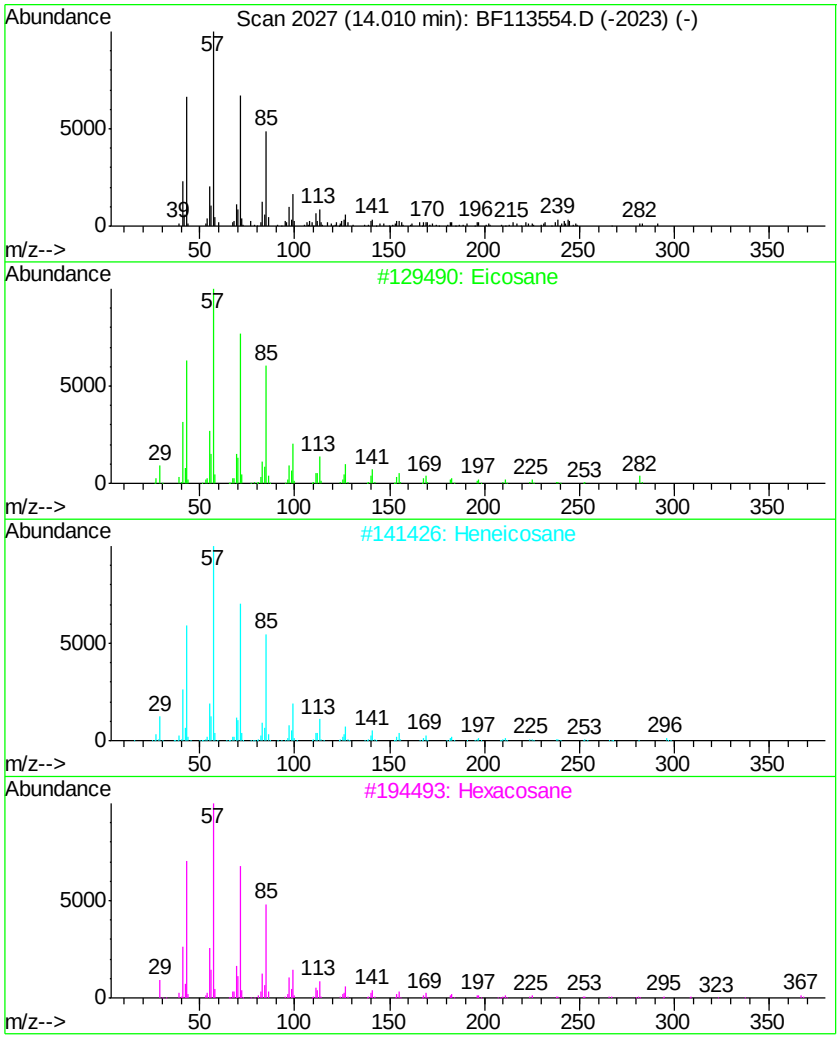
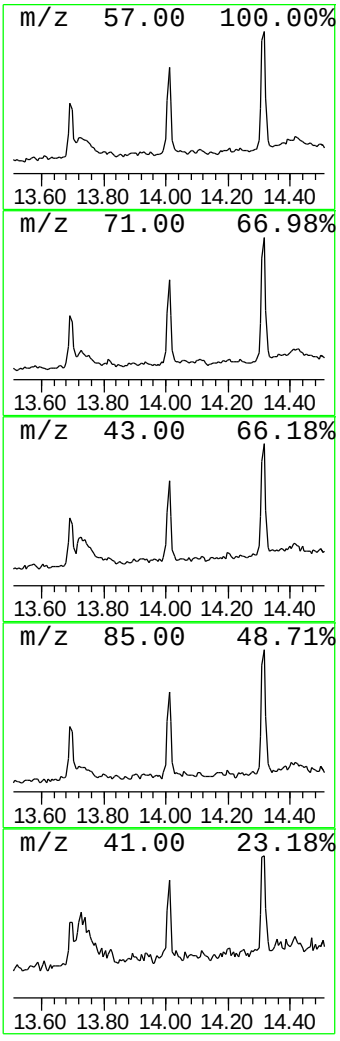
Peak Number 4 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.01	2.28 ng	111514	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Heneicosane	296	C21H44	000629-94-7	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Heptadecane	240	C17H36	000629-78-7	83





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040319\
Data File : BF113554.D
Acq On : 3 Apr 2019 20:16
Operator : JU/SJ
Sample : K2213-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S9A-S9B-S9C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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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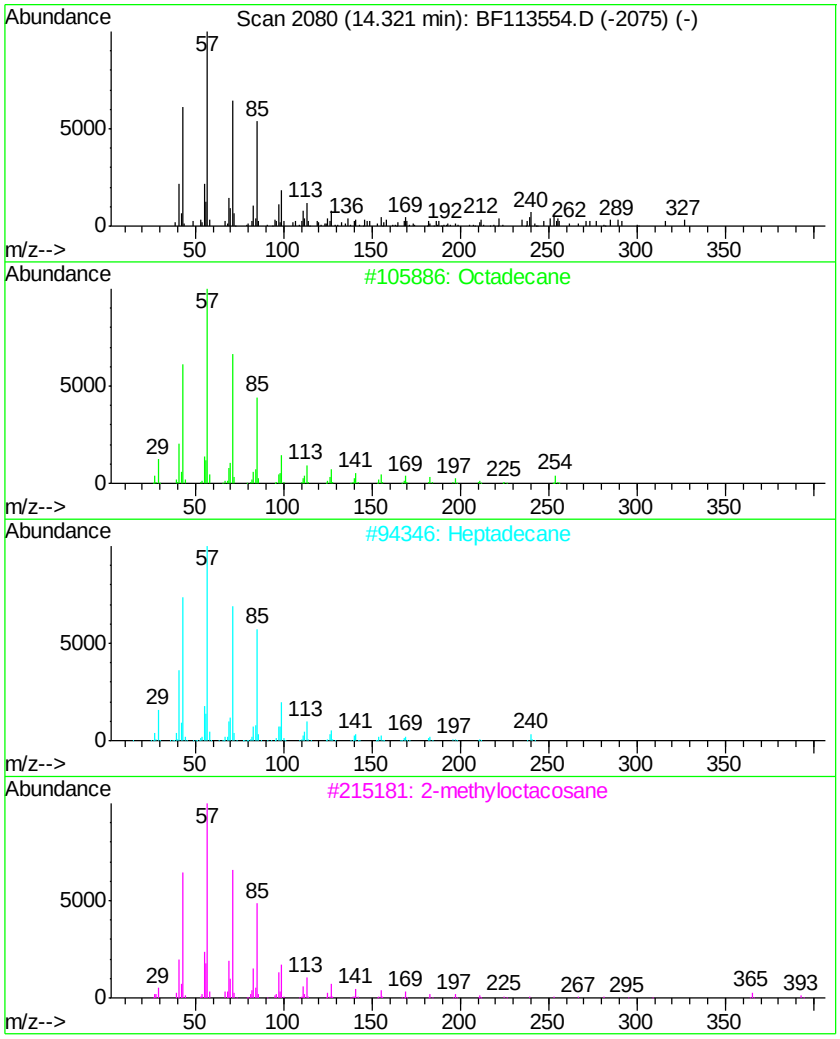
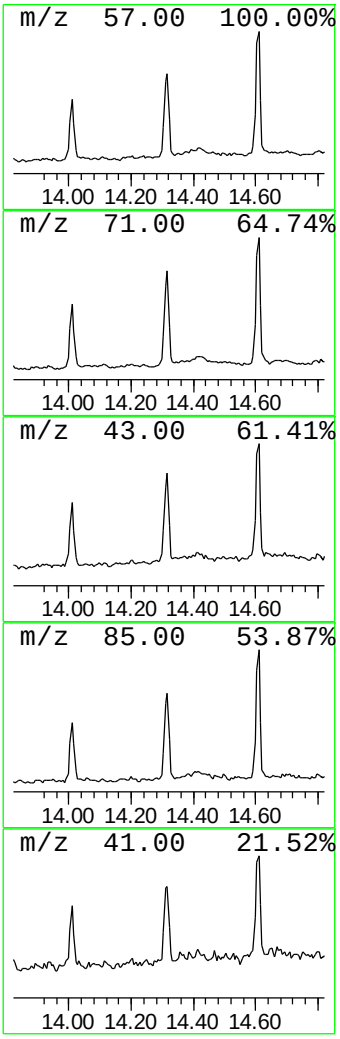
Peak Number 5 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.32	2.83 ng	138182	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	93
2	Heptadecane	240	C17H36	000629-78-7	93
3	2-methyloctacosane	408	C29H60	1000376-72-8	90
4	Tetracosane	338	C24H50	000646-31-1	90
5	Hexacosane	366	C26H54	000630-01-3	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040319\
Data File : BF113554.D
Acq On : 3 Apr 2019 20:16
Operator : JU/SJ
Sample : K2213-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S9A-S9B-S9C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

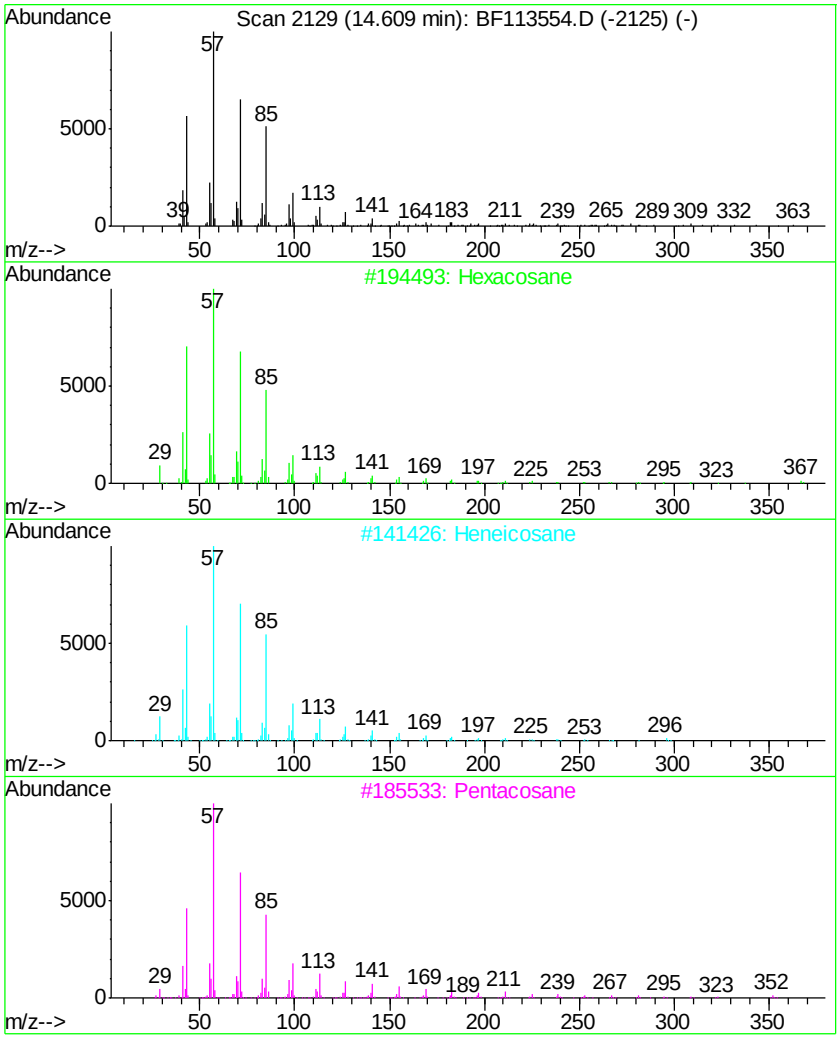
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

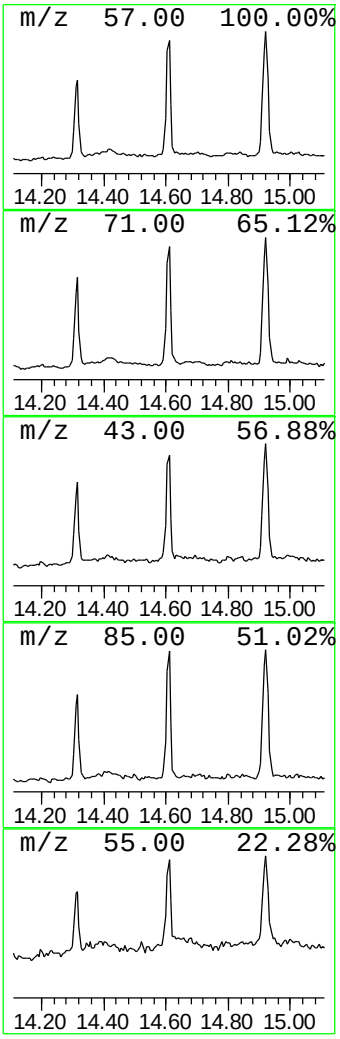
****

Peak Number 6 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	4.10 ng	204461	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Heneicosane	296	C21H44	000629-94-7	90
3	Pentacosane	352	C25H52	000629-99-2	87
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87
5	Hexadecane	226	C16H34	000544-76-3	83





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Data File : BF113554.D
Acq On : 3 Apr 2019 20:16
Operator : JU/SJ
Sample : K2213-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S9A-S9B-S9C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

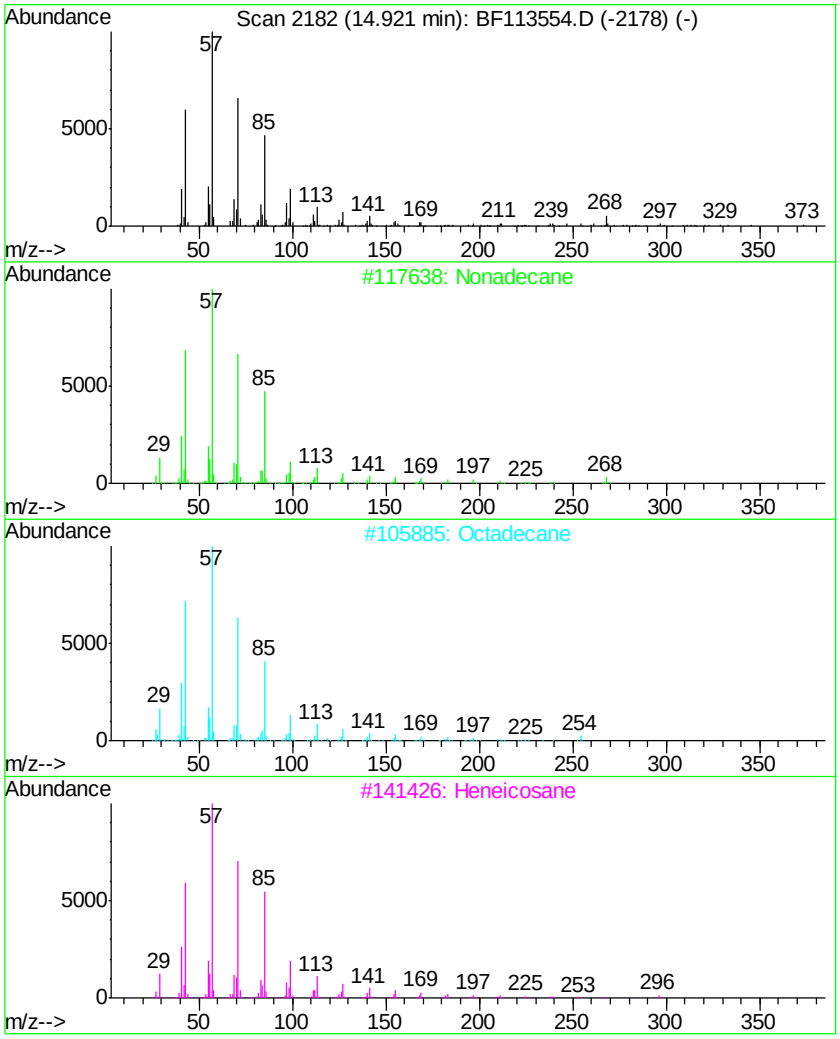
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

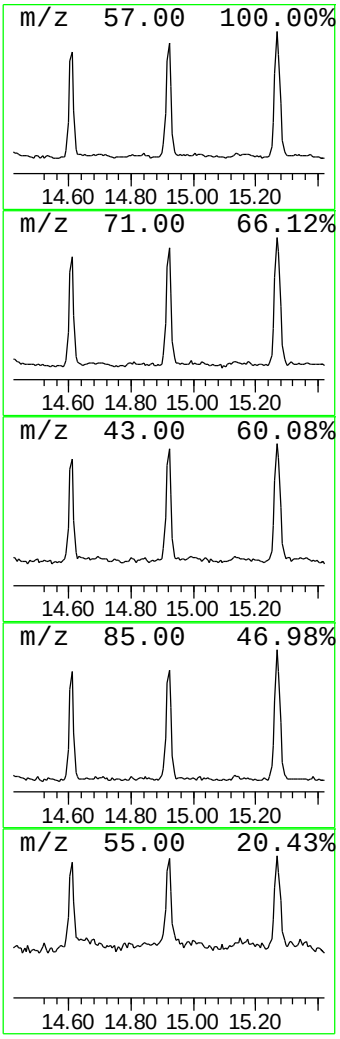
****

Peak Number 7 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	4.65 ng	231787	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	95
2	Octadecane	254	C18H38	000593-45-3	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Heptadecane	240	C17H36	000629-78-7	90
5	Tetracosane	338	C24H50	000646-31-1	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040319\
Data File : BF113554.D
Acq On : 3 Apr 2019 20:16
Operator : JU/SJ
Sample : K2213-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S9A-S9B-S9C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

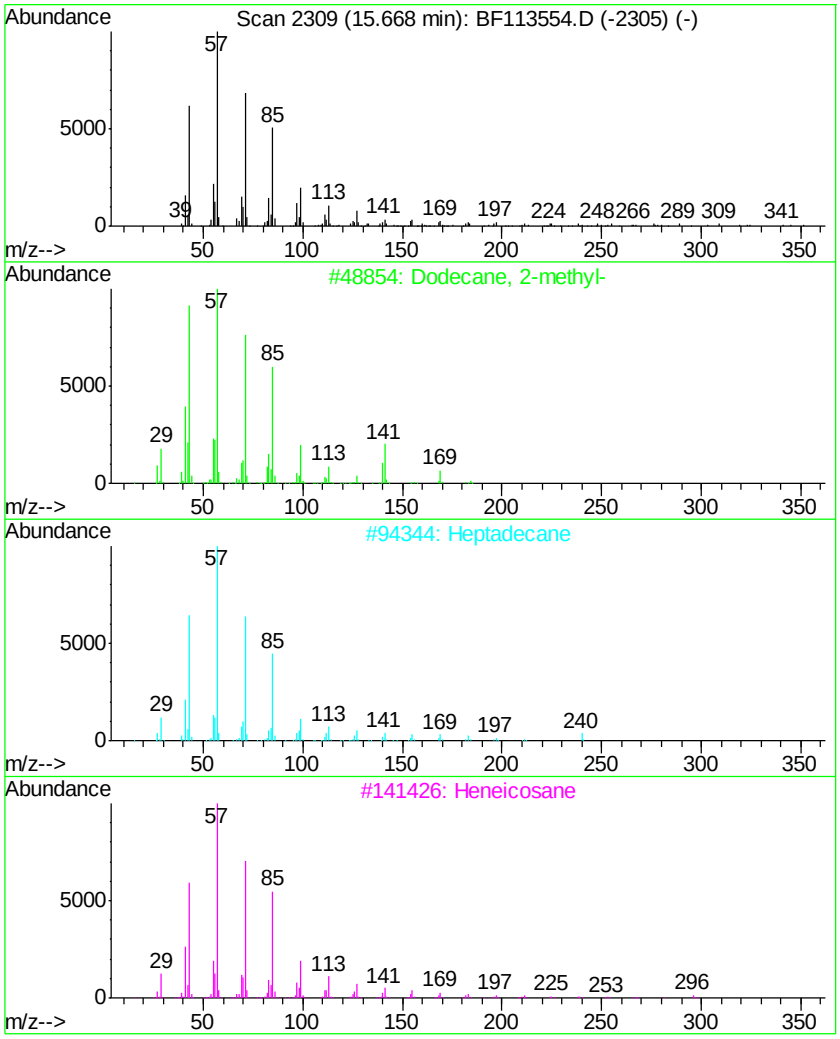
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

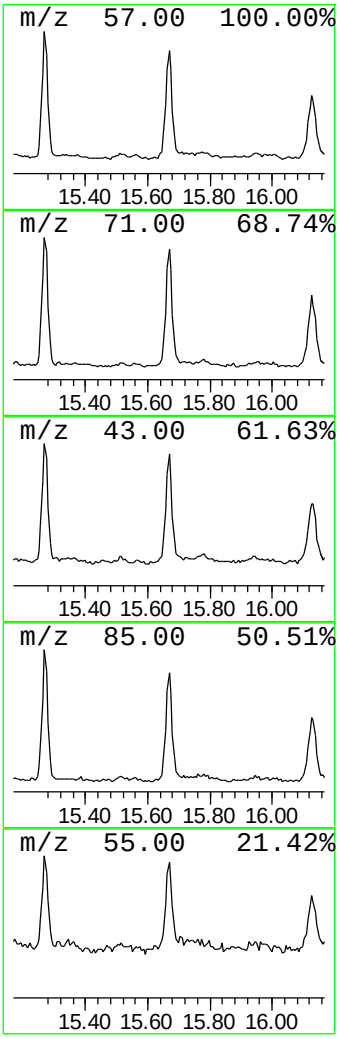
****

Peak Number 8 Dodecane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.67	5.29 ng	263695	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
2	Heptadecane	240	C17H36	000629-78-7	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	2-methyloctacosane	408	C29H60	1000376-72-8	87
5	Hexacosane	366	C26H54	000630-01-3	87





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Data File : BF113554.D
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Operator : JU/SJ
Sample : K2213-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S9A-S9B-S9C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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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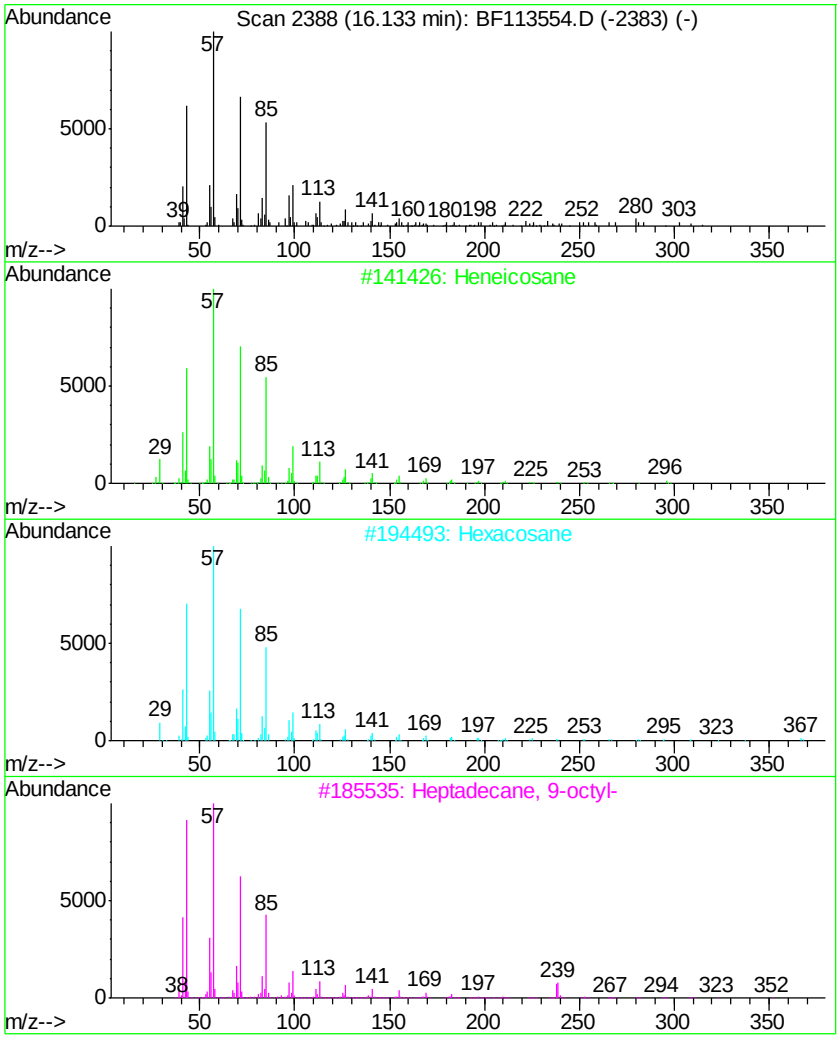
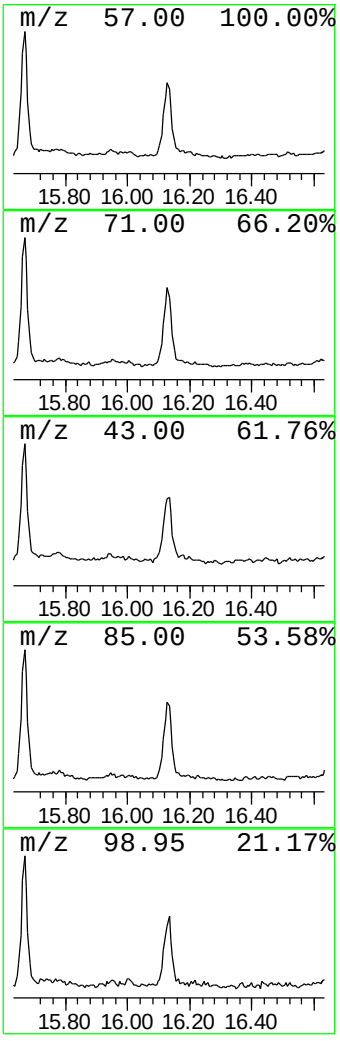
Peak Number 9 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	6.64 ng	331190	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Hexacosane	366	C26H54	000630-01-3	90
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4	Octacosane	394	C28H58	000630-02-4	87
5	2-methyloctacosane	408	C29H60	1000376-72-8	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040319\
Data File : BF113554.D
Acq On : 3 Apr 2019 20:16
Operator : JU/SJ
Sample : K2213-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S9A-S9B-S9C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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
unknown6.46	6.46	78.1	ng	2671340	1	6.69	684083	20.0
1,2-Benzenediol, ...	13.72	2.3	ng	113882	5	13.84	977015	20.0
Eicosane	14.01	2.3	ng	111514	5	13.84	977015	20.0
Octadecane	14.32	2.8	ng	138182	5	13.84	977015	20.0
Hexacosane	14.61	4.1	ng	204461	6	15.25	997002	20.0
Nonadecane	14.92	4.7	ng	231787	6	15.25	997002	20.0
Dodecane, 2-methyl-	15.67	5.3	ng	263695	6	15.25	997002	20.0
Heneicosane	16.13	6.6	ng	331190	6	15.25	997002	20.0