Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022119\
Data File : BF112650.D
Acq On : 21 Feb 2019 14:08
Operator : JU/SJ
Sample : K1547-03 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-S

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-BF012519.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	5.034	497	501	511	rBV	18574	29917	2.72%	0.221%
2	5.457	570	573	601	rBV	459055	684779	62.30%	5.051%
3	6.475	743	746	764	rBV	504675	772192	70.26%	5.696%
4	6.598	764	767	775	rBV	867135	836831	76.14%	6.173%
5	6.822	801	805	816	rBV	547640	546889	49.76%	4.034%
6	6.975	827	831	849	rBV	732852	668044	60.78%	4.928%
7	7.387	898	901	917	rBV	404062	510529	46.45%	3.766%
8	8.104	1019	1023	1039	rVB	703546	742827	67.59%	5.479%
9	8.687	1117	1122	1126	rVB2	18063	17619	1.60%	0.130%
10	9.175	1201	1205	1215	rBV	1198817	1099089	100.00%	8.107%
11	9.251	1215	1218	1221	rVB	21057	20856	1.90%	0.154%
12	9.575	1267	1273	1280	rBV	57456	64402	5.86%	0.475%
13	9.781	1305	1308	1313	rVB	16313	13737	1.25%	0.101%
14	9.857	1317	1321	1331	rBV	975578	908581	82.67%	6.702%
15	10.275	1389	1392	1395	rVB2	19207	15199	1.38%	0.112%
16	10.498	1425	1430	1433	rBV3	8695	11923	1.08%	0.088%
17	10.657	1453	1457	1471	rBV	594441	706898	64.32%	5.214%
18	10.751	1471	1473	1478	rVB3	16622	20696	1.88%	0.153%
19	11.198	1541	1549	1551	rBV2	18753	19094	1.74%	0.141%
20	11.345	1571	1574	1584	rBV	930948	996632	90.68%	7.351%
21	11.863	1658	1662	1665	rBV3	63258	76111	6.92%	0.561%
22	11.969	1677	1680	1682	rBV2	14777	16467	1.50%	0.121%
23	12.027	1687	1690	1693	rBV	27405	19785	1.80%	0.146%
24	12.404	1751	1754	1755	rBV	12554	12725	1.16%	0.094%
25	12.569	1778	1782	1786	rBV	153229	158641	14.43%	1.170%
26	12.657	1794	1797	1804	rBV7	18062	39208	3.57%	0.289%
27	12.722	1804	1808	1813	rVV6	11475	19728	1.79%	0.146%
28	12.798	1814	1821	1827	rVV	147359	191428	17.42%	1.412%
29	12.927	1839	1843	1846	rBV	1114810	1071220	97.46%	7.901%
30	13.010	1853	1857	1862	rBV5	16267	26477	2.41%	0.195%
31	13.139	1877	1879	1882	rVB2	26195	25475	2.32%	0.188%
32	13.233	1891	1895	1899	rBV3	18515	24210	2.20%	0.179%
33	13.322	1908	1910	1913	rBV3	11204	13056	1.19%	0.096%
34	13.357	1913	1916	1918	rVV3	14484	13691	1.25%	0.101%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF022119\
Data File : BF112650.D
Acq On : 21 Feb 2019 14:08
Operator : JU/SJ
Sample : K1547-03 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-S

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-BF012519.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.480	1934	1937	1943	rBV	41423	55855	5.08%	0.412%
36	13.816	1990	1994	2000	rBV5	60892	100020	9.10%	0.738%
37	13.945	2014	2016	2018	rVB	20849	16816	1.53%	0.124%
38	13.992	2020	2024	2028	rBV	730198	830690	75.58%	6.127%
39	14.127	2044	2047	2050	rVB	99979	88892	8.09%	0.656%
40	14.433	2095	2099	2101	rBV2	141860	148503	13.51%	1.095%
41	14.733	2146	2150	2154	rVB	163636	168254	15.31%	1.241%
42	14.804	2160	2162	2167	rVB2	34441	39379	3.58%	0.290%
43	15.063	2200	2206	2213	rVB2	180667	293122	26.67%	2.162%
44	15.345	2252	2254	2258	rVB	30072	32911	2.99%	0.243%
45	15.433	2262	2269	2272	rBV2	168331	279059	25.39%	2.058%
46	15.468	2272	2275	2287	rVB	518717	686087	62.42%	5.061%
47	15.857	2336	2341	2347	rBV	129369	202116	18.39%	1.491%
48	16.351	2420	2425	2431	rVB2	88690	160516	14.60%	1.184%
49	16.927	2519	2523	2528	rBV	32080	60214	5.48%	0.444%

Sum of corrected areas: 13557390

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022119\
Data File : BF112650.D
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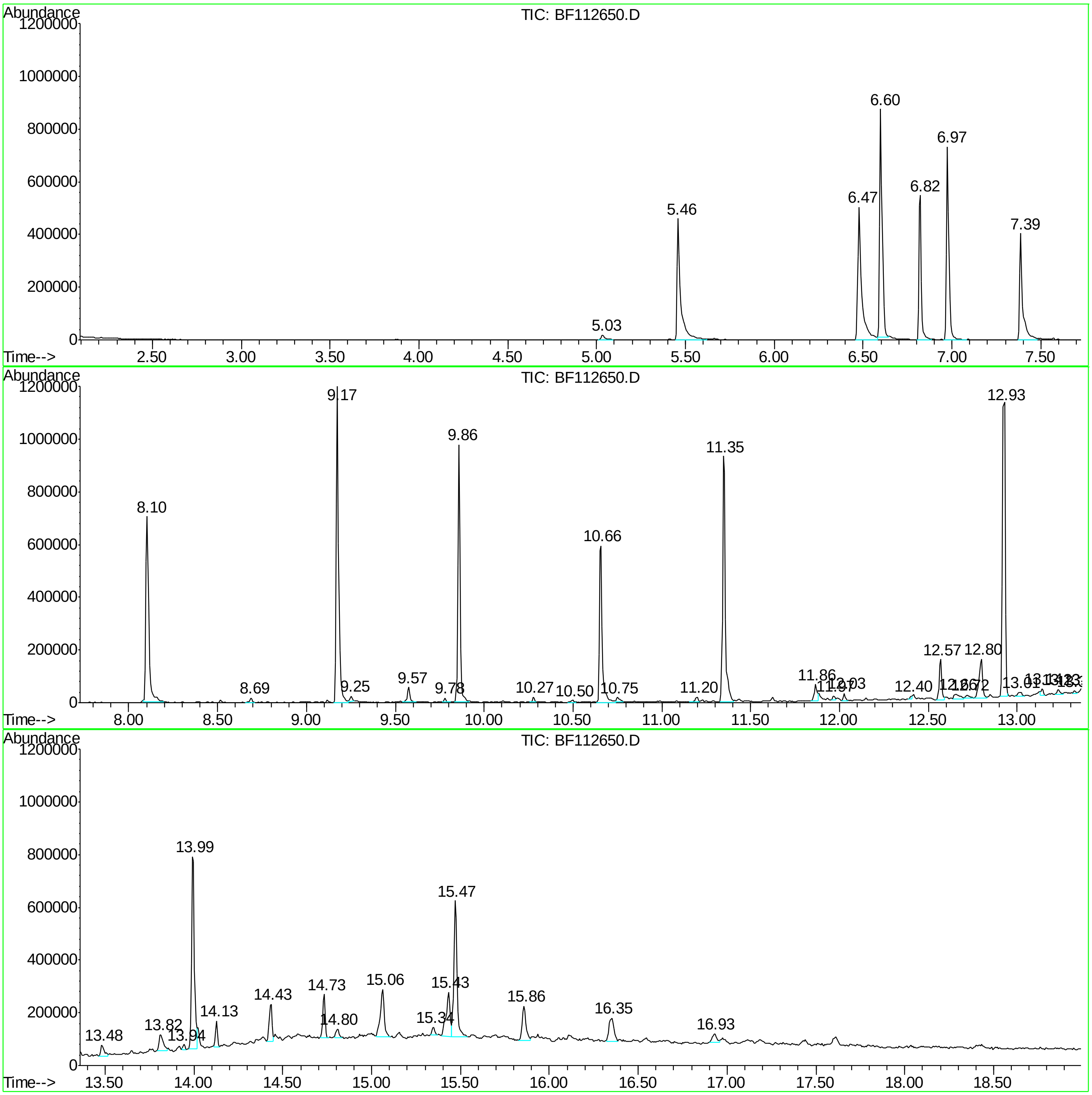
Sample : K1547-03 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Instrument :
BNA_F
ClientSampleId :
TP-1-S



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022119\
Data File : BF112650.D
Acq On : 21 Feb 2019 14:08
Operator : JU/SJ
Sample : K1547-03 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

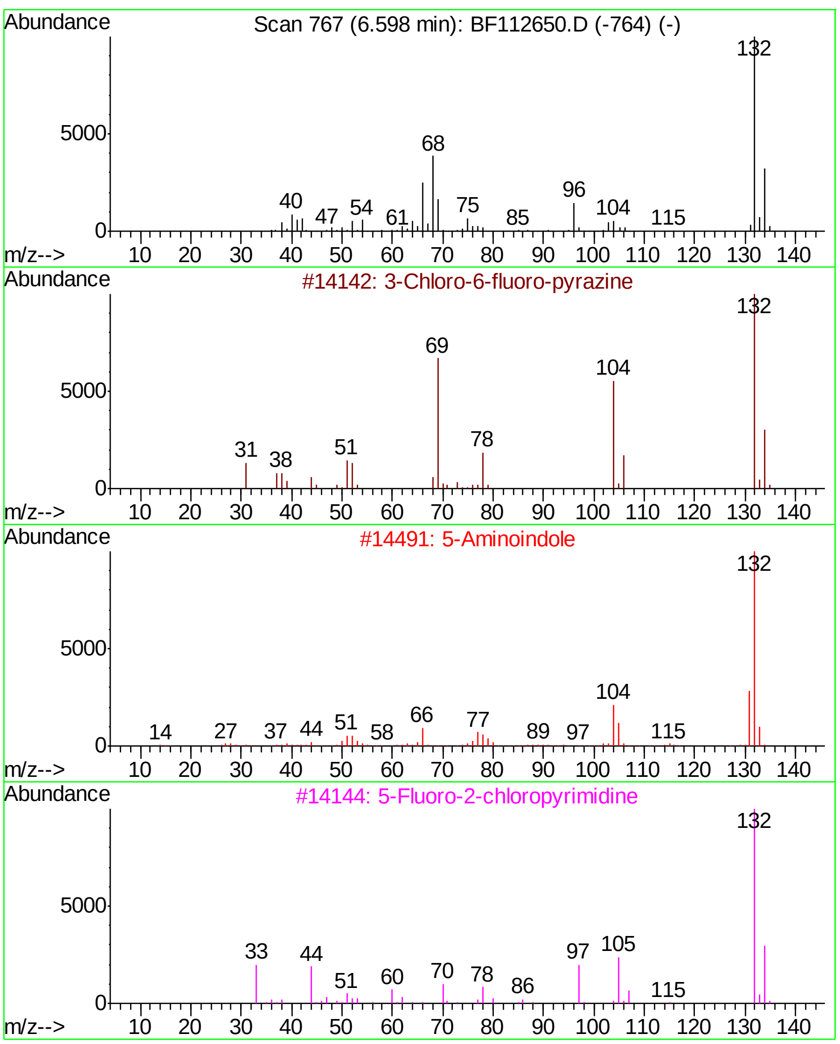
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

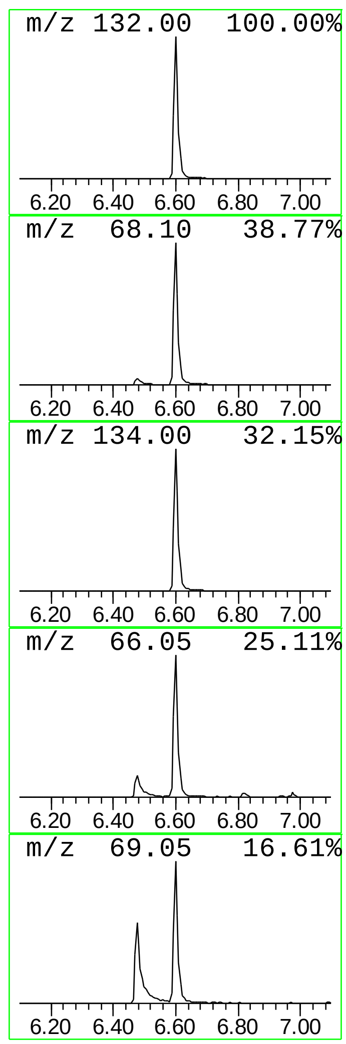
****

Peak Number 1 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	30.60 ng	836831	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022119\
Data File : BF112650.D
Acq On : 21 Feb 2019 14:08
Operator : JU/SJ
Sample : K1547-03 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

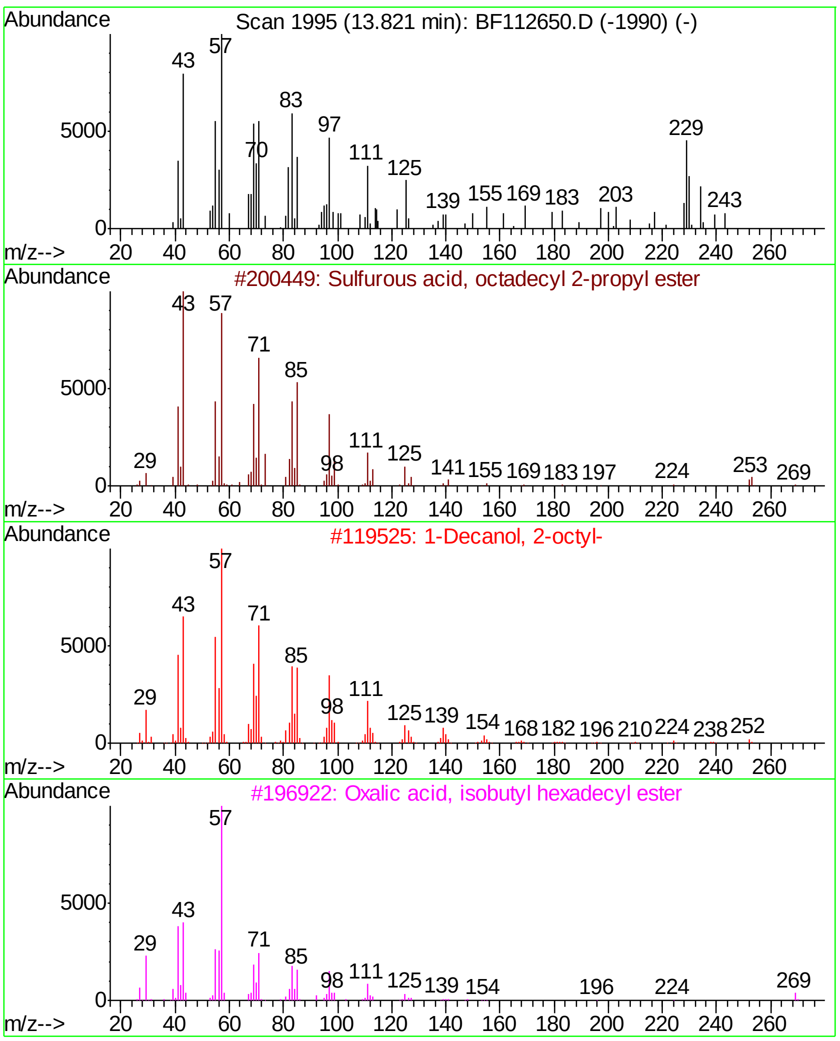
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

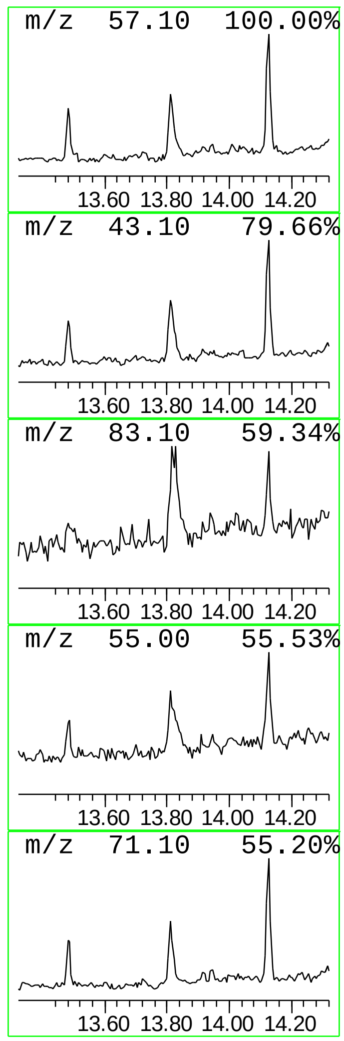
****

Peak Number 3 Sulfurous acid, octadecyl 2... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	2.41 ng	100020	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	76
2	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	68
3	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	64
4	Nonahexacontanoic acid	999	C69H138O2	040710-32-5	52
5	2-methyltetracosane	352	C25H52	1000376-72-6	43





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022119\
Data File : BF112650.D
Acq On : 21 Feb 2019 14:08
Operator : JU/SJ
Sample : K1547-03 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012519.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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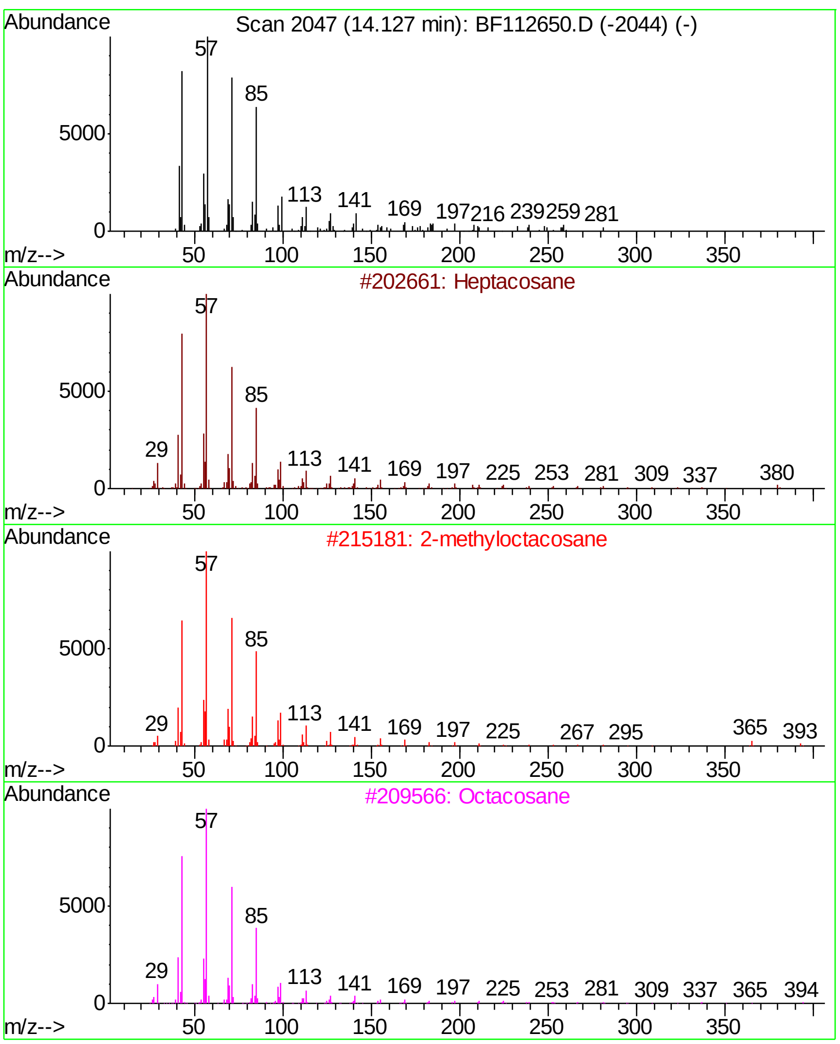
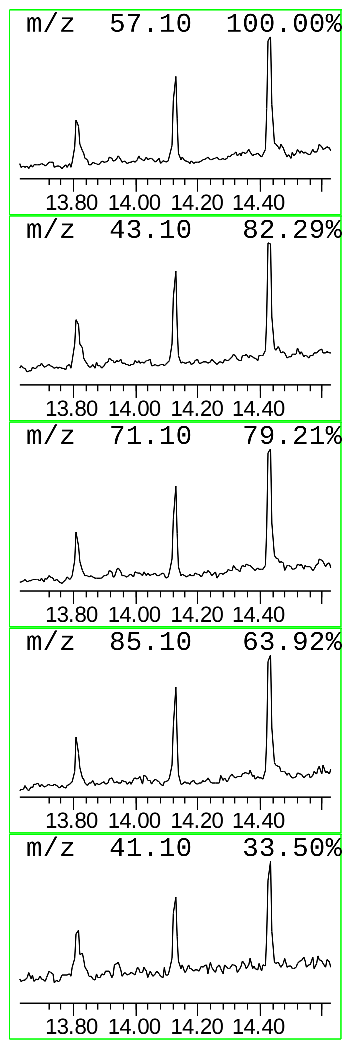
Peak Number 4 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.13	2.14 ng	88892	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	$C_{27}H_{56}$	000593-49-7	91
2	2-methyloctacosane	408	$C_{29}H_{60}$	1000376-72-8	91
3	Octacosane	394	$C_{28}H_{58}$	000630-02-4	91
4	Pentacosane	352	$C_{25}H_{52}$	000629-99-2	91
5	Triacontane	422	$C_{30}H_{62}$	000638-68-6	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022119\
Data File : BF112650.D
Acq On : 21 Feb 2019 14:08
Operator : JU/SJ
Sample : K1547-03 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012519.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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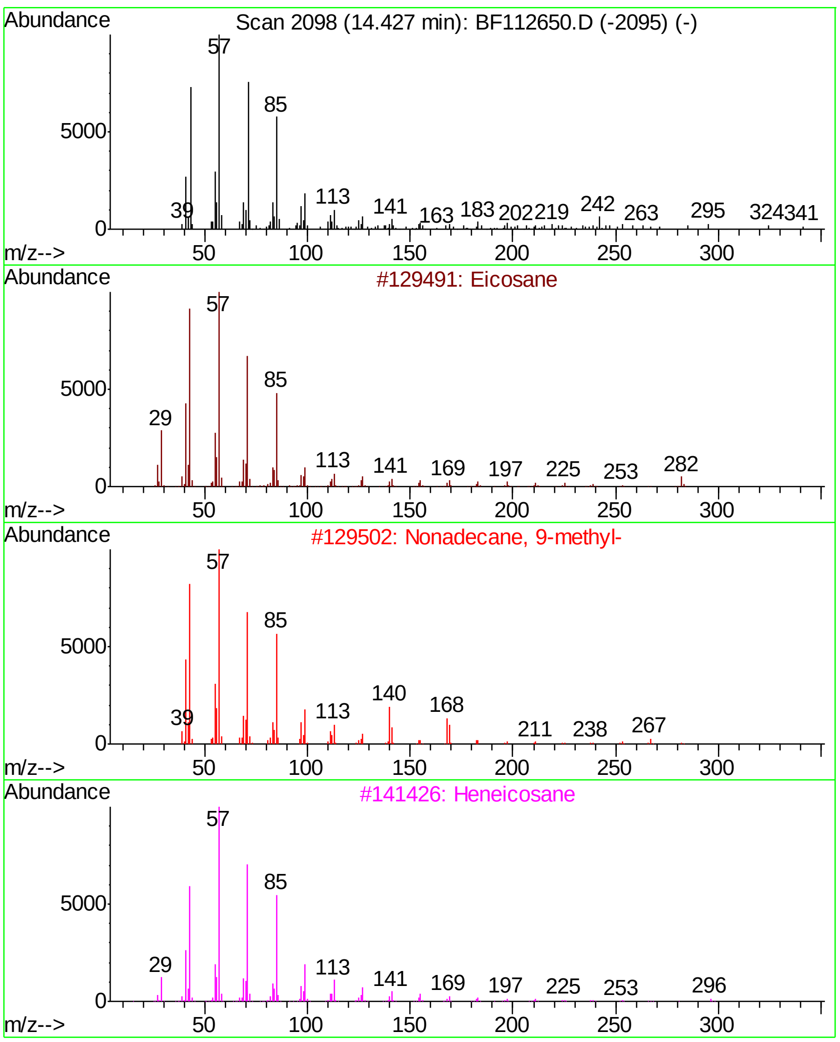
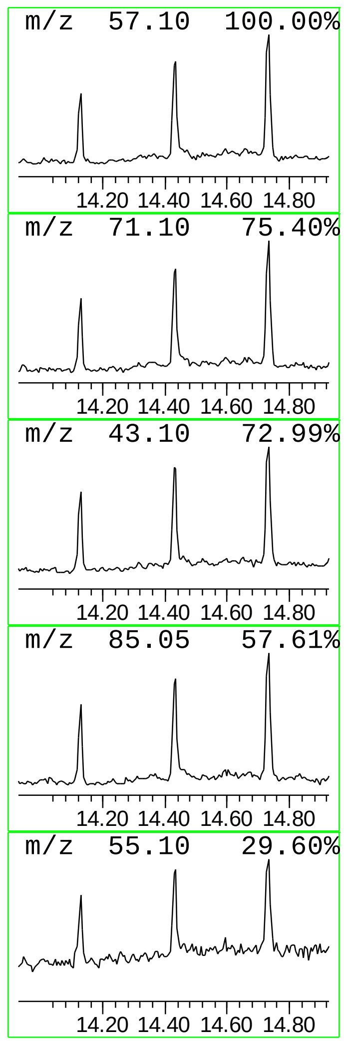
Peak Number 5 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	3.58 ng	148503	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	92
3	Heneicosane	296	C21H44	000629-94-7	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022119\
Data File : BF112650.D
Acq On : 21 Feb 2019 14:08
Operator : JU/SJ
Sample : K1547-03 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012519.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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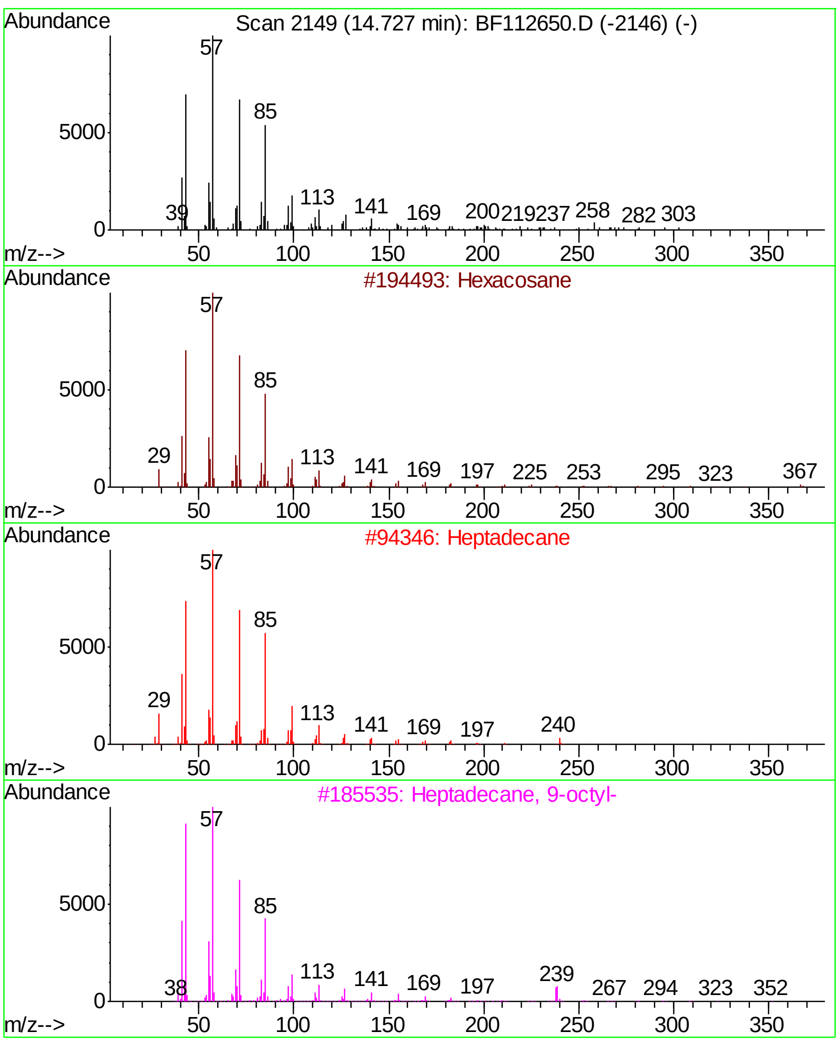
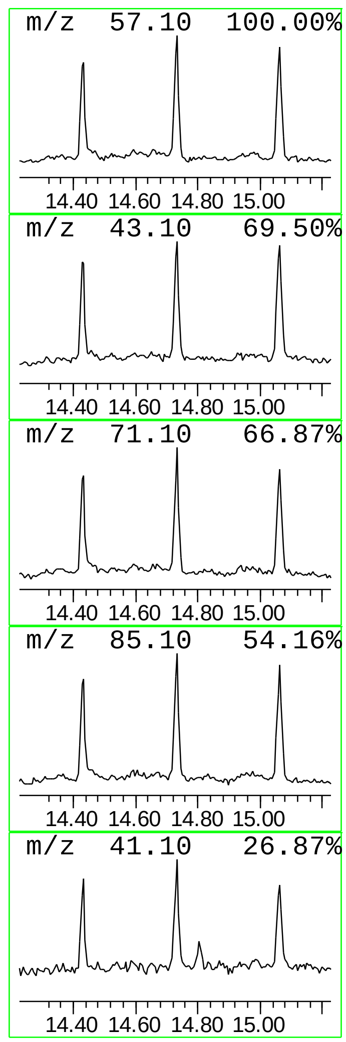
Peak Number 6 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	4.05 ng	168254	Chrysene-d12	14.00

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





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022119\
Data File : BF112650.D
Acq On : 21 Feb 2019 14:08
Operator : JU/SJ
Sample : K1547-03 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012519.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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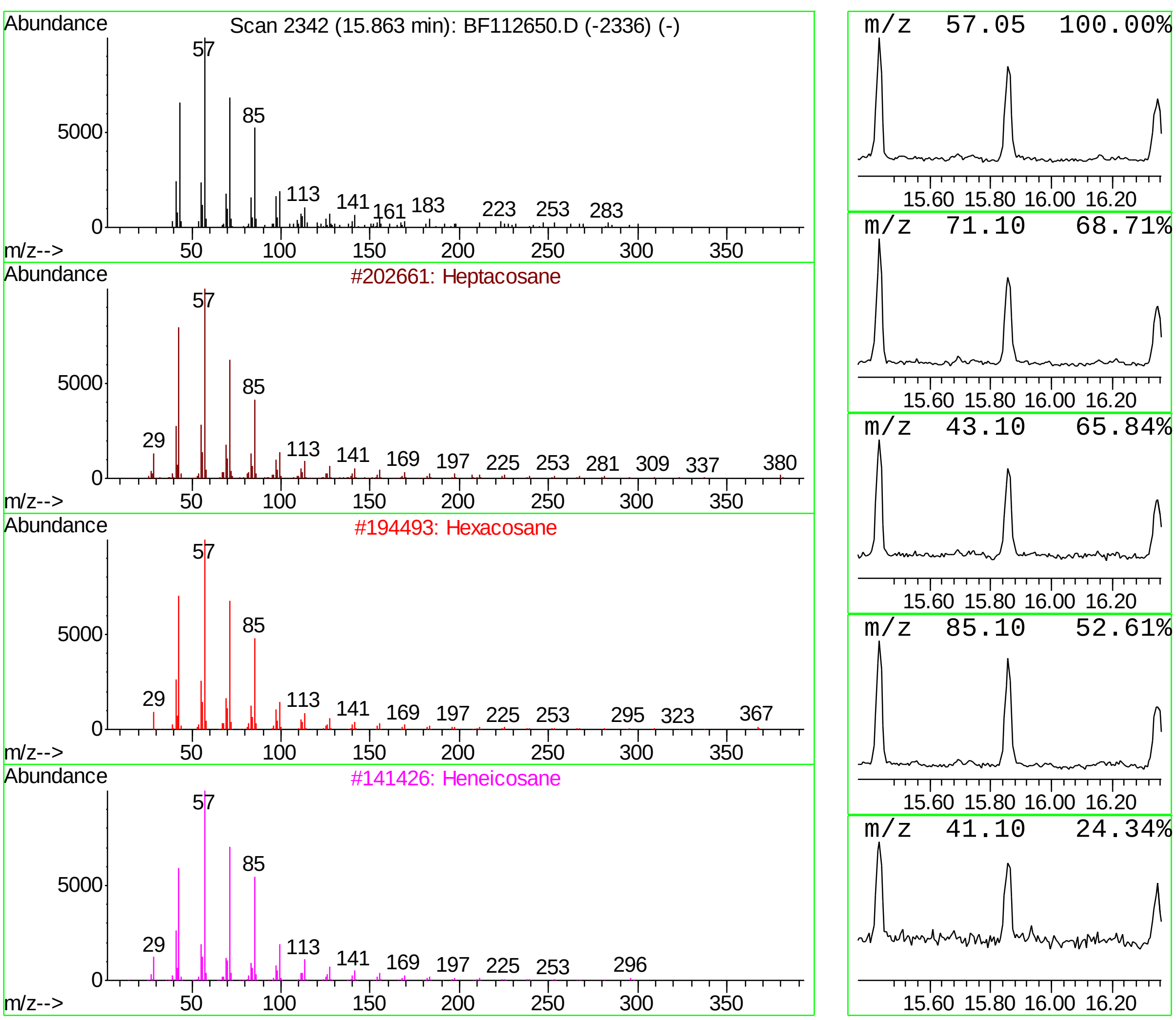
Peak Number 7 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	5.89 ng	202116	Perylene-d12	15.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	$C_{27}H_{56}$	000593-49-7	91
2	Hexacosane	366	$C_{26}H_{54}$	000630-01-3	90
3	Heneicosane	296	$C_{21}H_{44}$	000629-94-7	90
4	Hentriacontane	437	$C_{31}H_{64}$	000630-04-6	89
5	Sulfurous acid, butyl undecyl ester	292	$C_{15}H_{32}O_3S$	1000309-17-8	87



Library Search Compound Report

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Data File : BF112650.D
Acq On    : 21 Feb 2019  14:08
Operator  : JU/SJ
Sample    : K1547-03 2X
Misc      :
ALS Vial  : 7   Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012519.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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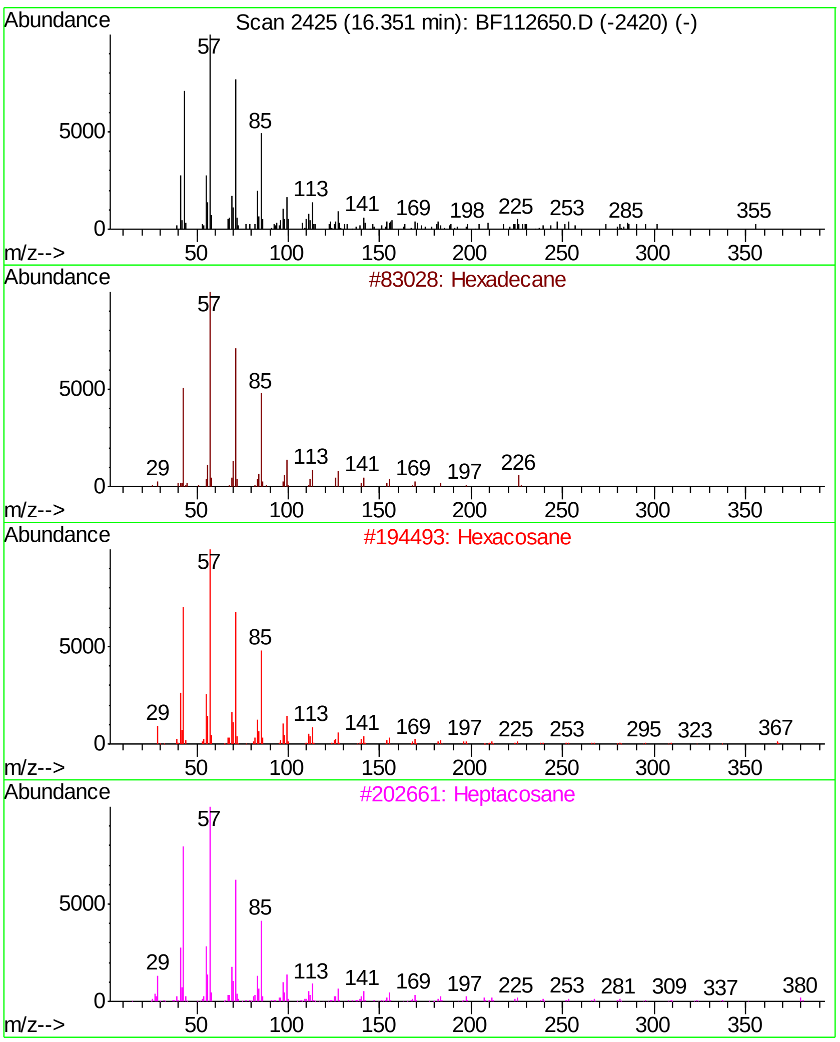
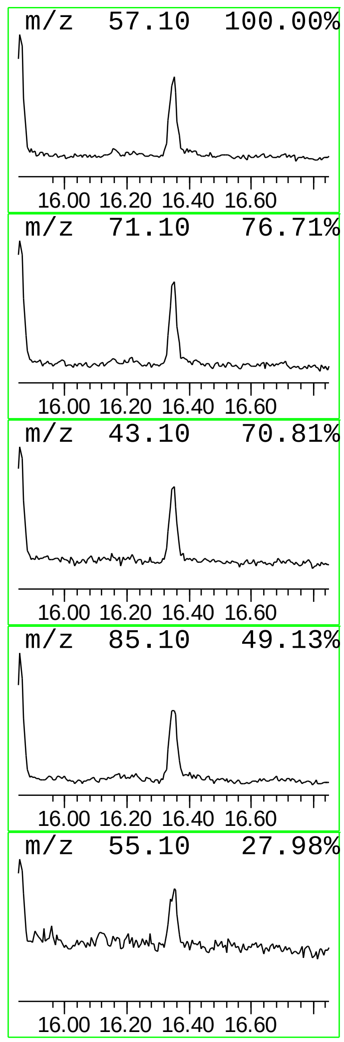
Instrument : BNA_F
ClientSampleId : TP-1-S

```
*********************************************************************
Peak Number  8  Hexadecane                      Concentration Rank  4
```

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.35	4.68 ng	160516	Perylene-d12	15.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	$C_{16}H_{34}$	000544-76-3	95
2	Hexacosane	366	$C_{26}H_{54}$	000630-01-3	90
3	Heptacosane	380	$C_{27}H_{56}$	000593-49-7	87
4	Heptadecane, 9-octyl-	352	$C_{25}H_{52}$	007225-64-1	87
5	Tetratetracontane	619	$C_{44}H_{90}$	007098-22-8	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF022119\
Data File : BF112650.D
Acq On : 21 Feb 2019 14:08
Operator : JU/SJ
Sample : K1547-03 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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
unknown6.60	6.60	30.6	ng	836831	1	6.82	546889	20.0
Sulfurous acid, o...	13.82	2.4	ng	100020	5	14.00	830690	20.0
Heptacosane	14.13	2.1	ng	88892	5	14.00	830690	20.0
Eicosane	14.43	3.6	ng	148503	5	14.00	830690	20.0
Hexacosane	14.73	4.0	ng	168254	5	14.00	830690	20.0
Heneicosane	15.86	5.9	ng	202116	6	15.47	686087	20.0
Hexadecane	16.35	4.7	ng	160516	6	15.47	686087	20.0