LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090619\
Data File : BF116863.D
Acq On : 6 Sep 2019 15:53
Operator : HP/JU
Sample : K4650-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-6

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-BF083019.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	2.110	3	4	16	rVB	320425	334255	19.30%	2.177%
2	5.469	570	575	578	rBV	1532094	1373991	79.32%	8.949%
3	6.481	742	747	760	rBV	1629802	1551647	89.57%	10.106%
4	6.616	766	770	773	rBV	1791137	1555136	89.78%	10.129%
5	6.845	806	809	817	rBV	558835	444354	25.65%	2.894%
6	7.004	832	836	839	rBV	1426718	1154940	66.67%	7.522%
7	7.404	899	904	907	rBV	1067882	912275	52.66%	5.942%
8	8.128	1023	1027	1044	rBV	672873	586069	33.83%	3.817%
9	9.198	1205	1209	1220	rBV	1978280	1732244	100.00%	11.282%
10	9.316	1226	1229	1234	rVB	53499	45016	2.60%	0.293%
11	9.592	1272	1276	1285	rBV	269858	255092	14.73%	1.661%
12	9.880	1321	1325	1336	rVB	799246	664828	38.38%	4.330%
13	10.669	1455	1459	1474	rVB	915391	872237	50.35%	5.681%
14	11.363	1573	1577	1584	rBV	740393	614287	35.46%	4.001%
15	11.886	1662	1666	1676	rBV	135390	129507	7.48%	0.843%
16	12.404	1750	1754	1759	rBV2	39743	50507	2.92%	0.329%
17	12.669	1796	1799	1804	rBV2	33685	36461	2.10%	0.237%
18	12.945	1841	1846	1849	rBV	1662162	1414388	81.65%	9.212%
19	13.516	1938	1943	1945	rBV4	20431	26095	1.51%	0.170%
20	13.833	1994	1997	2007	rBV	187992	249206	14.39%	1.623%
21	13.998	2021	2025	2028	rBV	476298	423001	24.42%	2.755%
22	14.157	2048	2052	2055	rBV	46508	45599	2.63%	0.297%
23	14.463	2101	2104	2110	rBV2	59164	58961	3.40%	0.384%
24	14.762	2152	2155	2160	rVB	64280	72034	4.16%	0.469%
25	14.839	2165	2168	2172	rVB	23221	23261	1.34%	0.152%
26	15.104	2208	2213	2217	rBV	69953	87814	5.07%	0.572%
27	15.457	2268	2273	2281	rVB	389068	531010	30.65%	3.459%
28	15.909	2345	2350	2354	rBV	50300	73702	4.25%	0.480%
29	16.404	2431	2434	2440	rVB3	23462	35810	2.07%	0.233%

Sum of corrected areas: 15353727

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Operator : HP/JU
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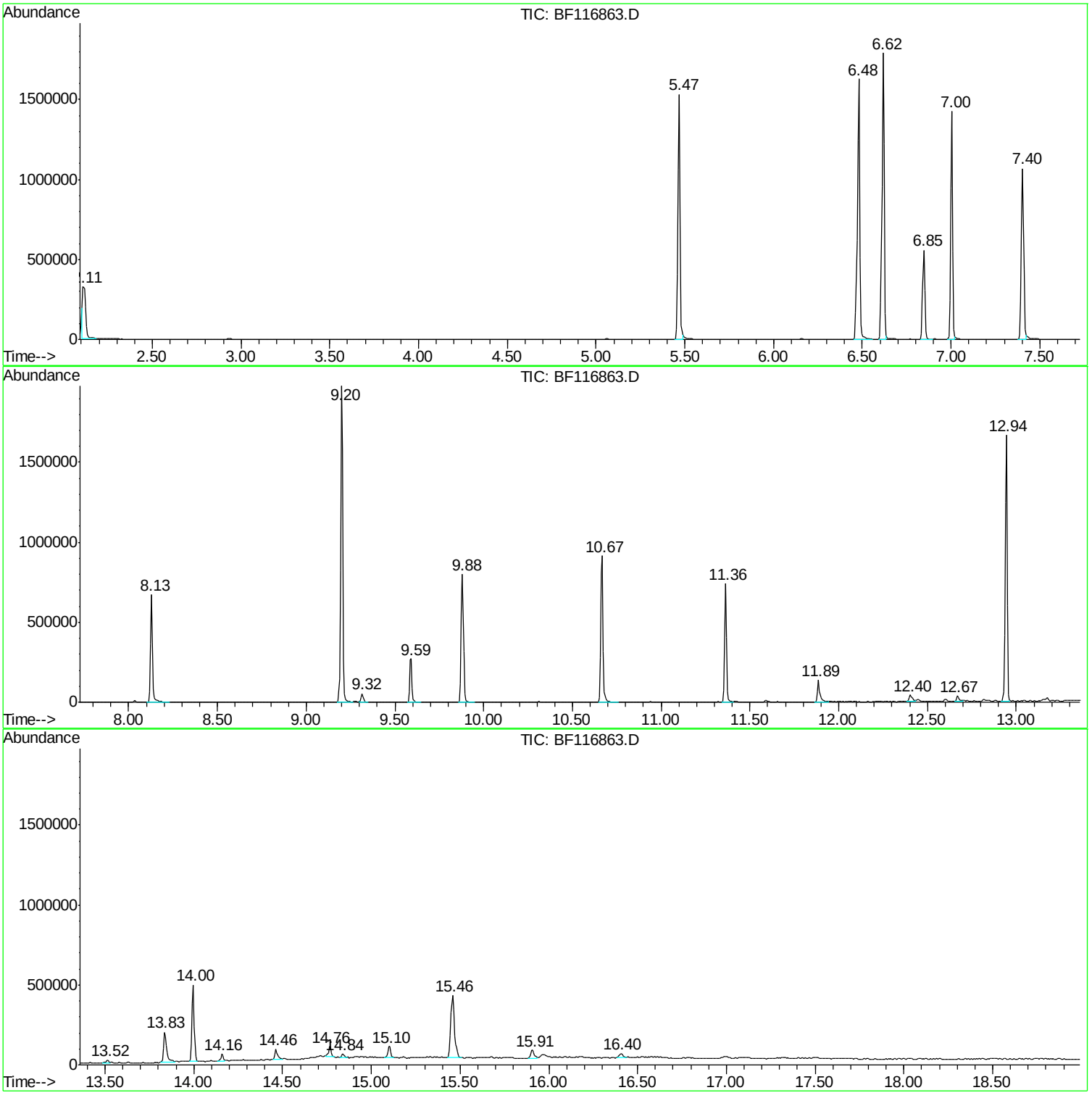
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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\BF090619\
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

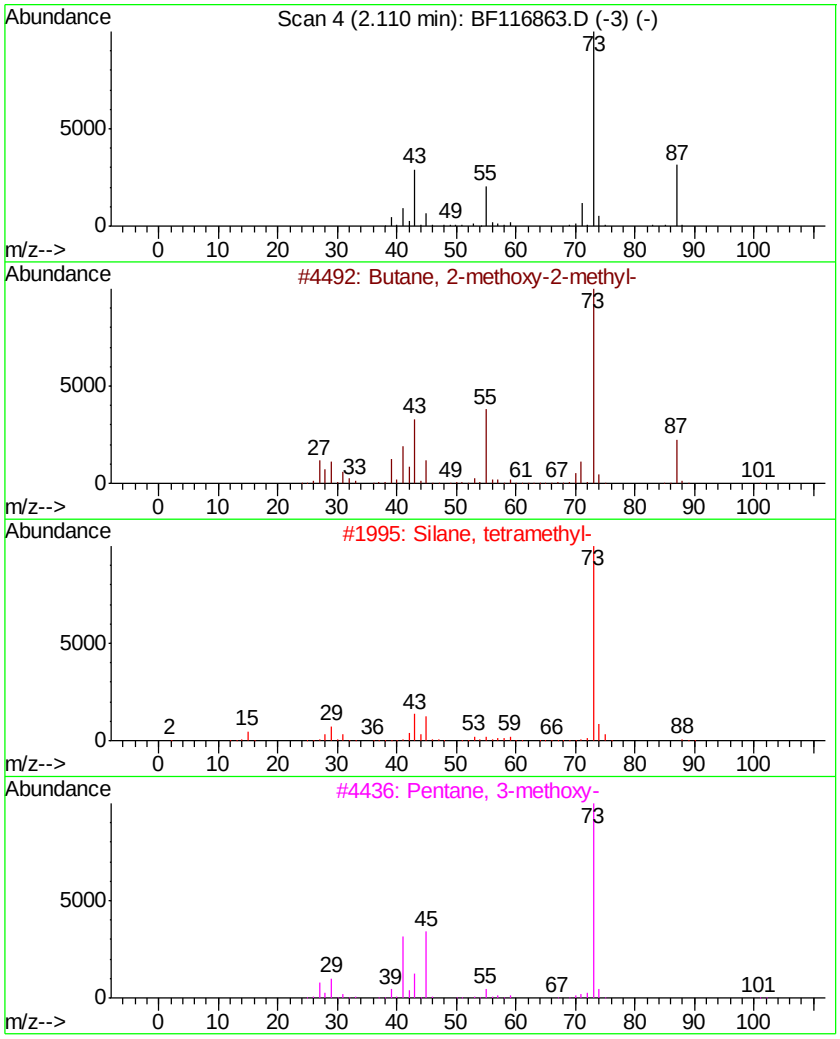
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

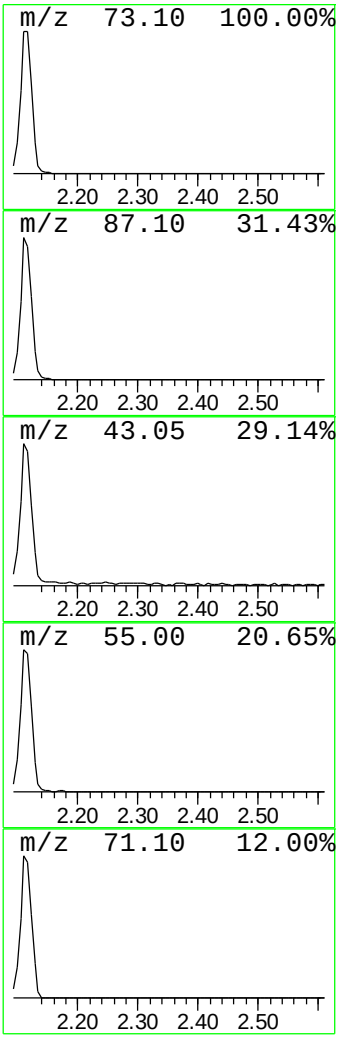
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.11	15.04 ng	334255	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	9





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Operator : HP/JU
Sample : K4650-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

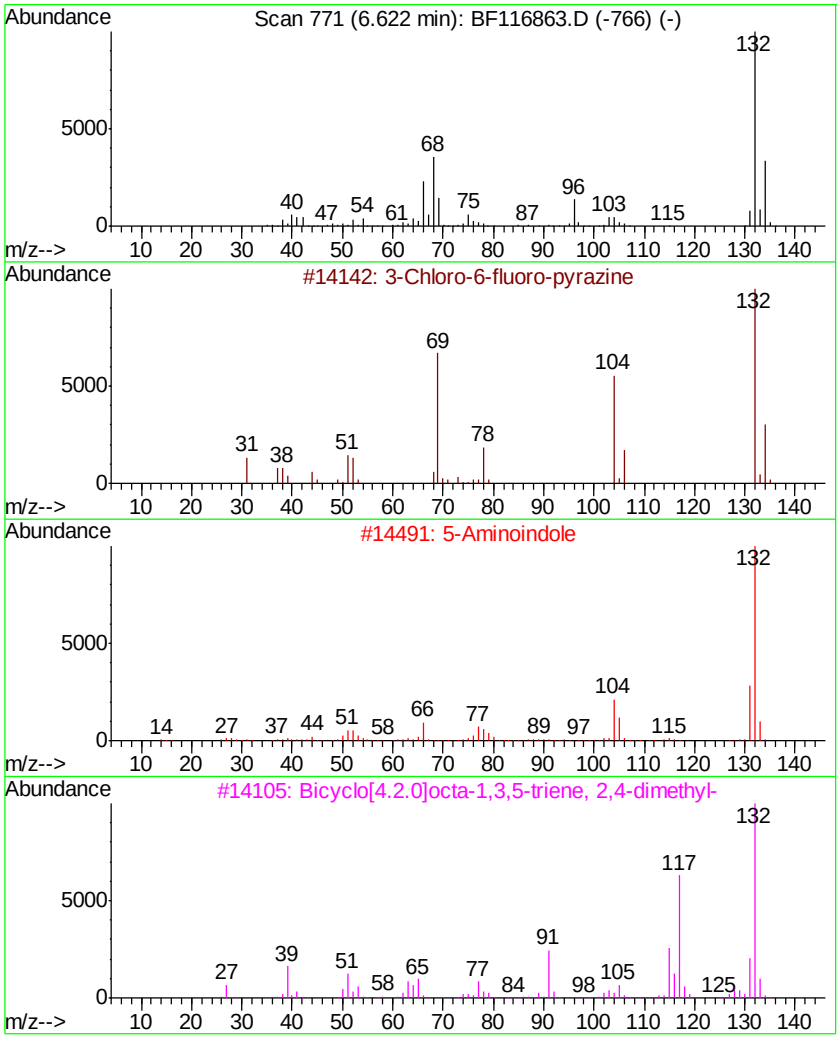
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

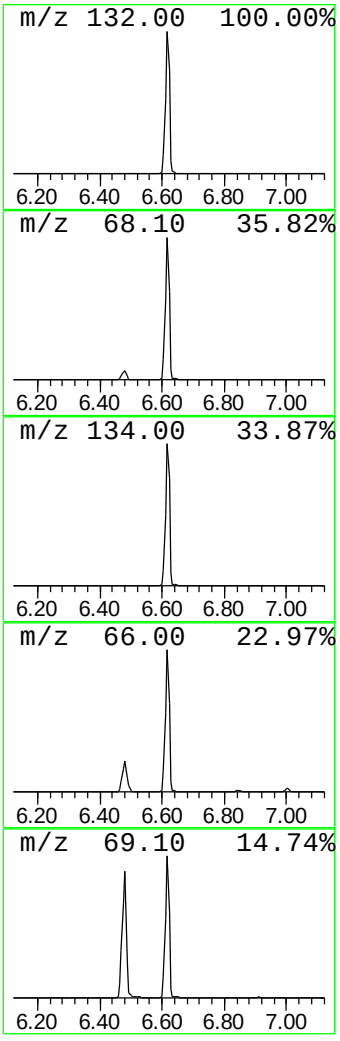
****

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	70.00 ng	1555140	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	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	10
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	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Library Search Compound Report

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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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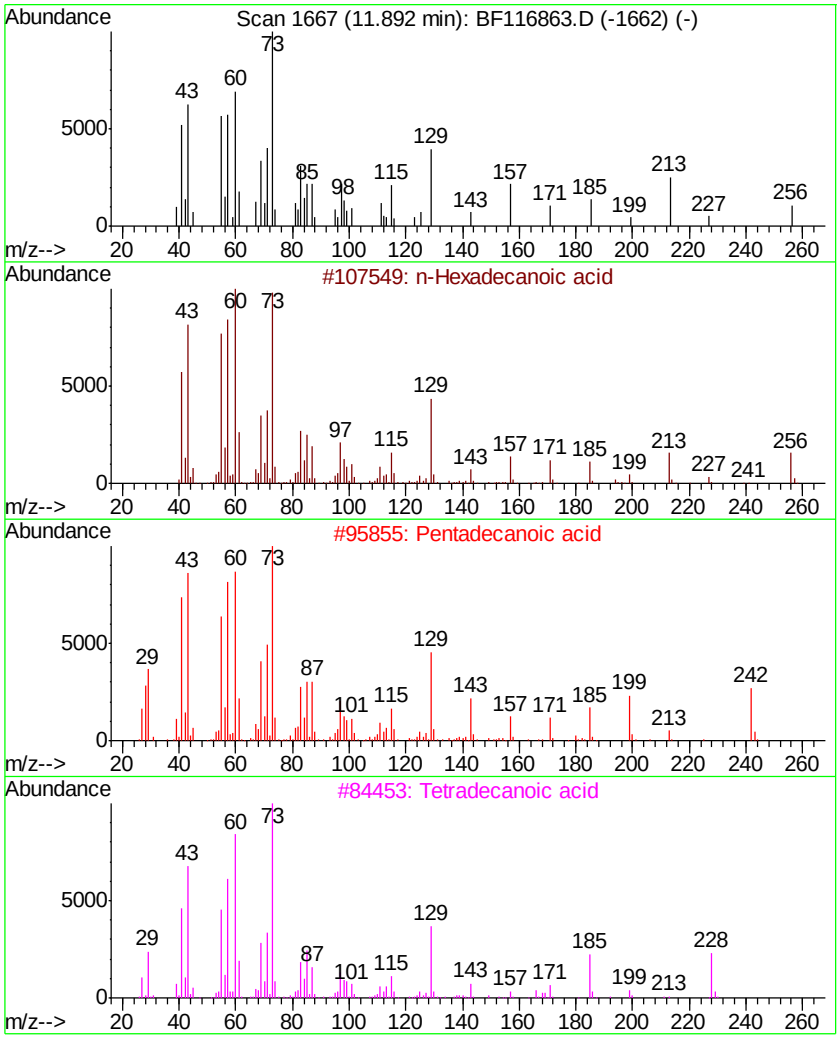
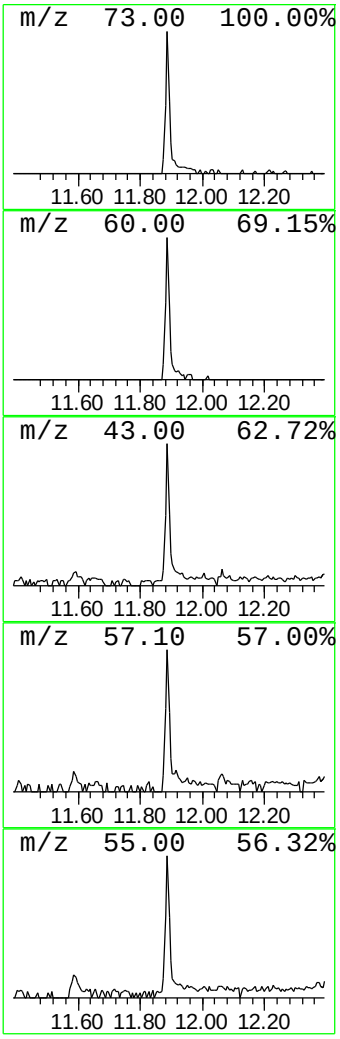
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	4.22 ng	129507	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	25





Library Search Compound Report

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Data File : BF116863.D
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Operator : HP/JU
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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

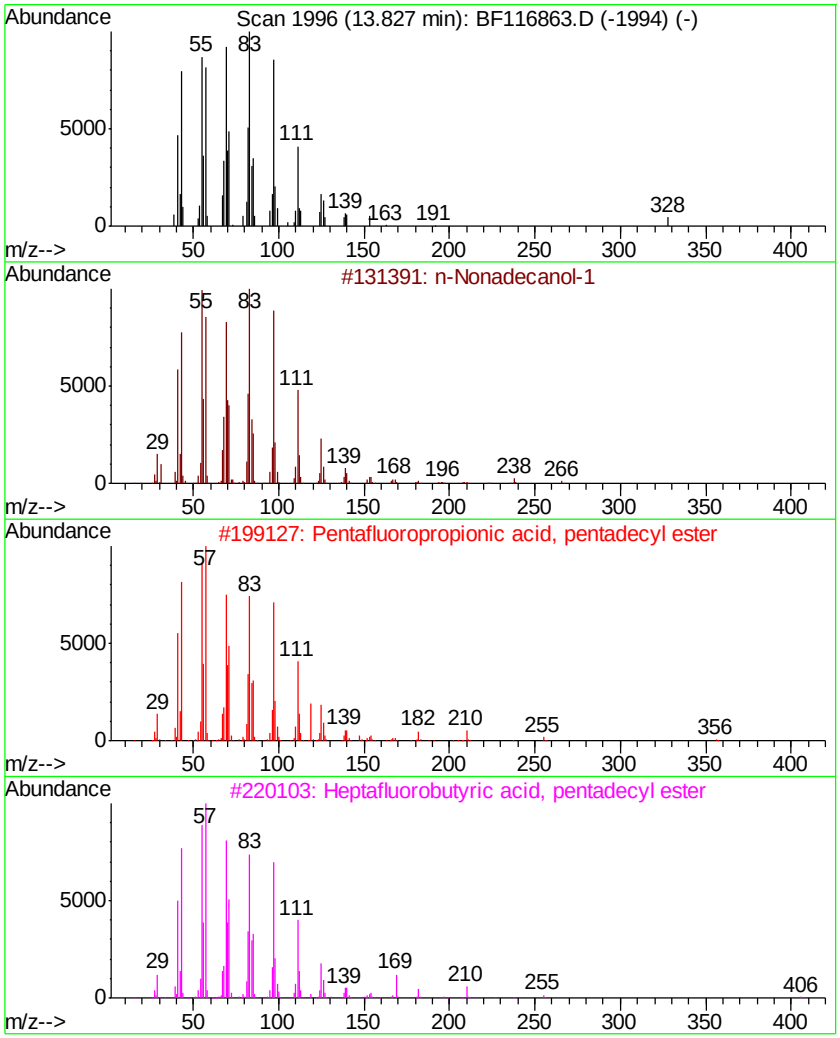
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

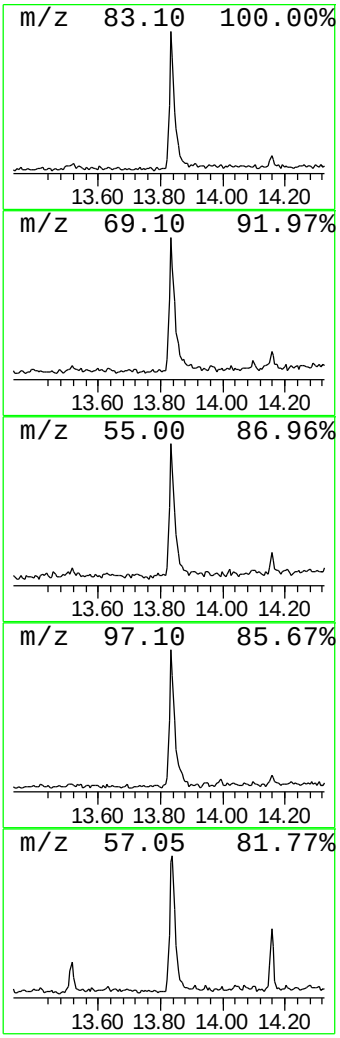
****

Peak Number 5 n-Nonadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	11.78 ng	249206	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
5	1-Heneicosanol	312	C21H44O	015594-90-8	91





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Sample : K4650-11
Misc :
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Instrument : BNA_F
ClientSampleId : TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

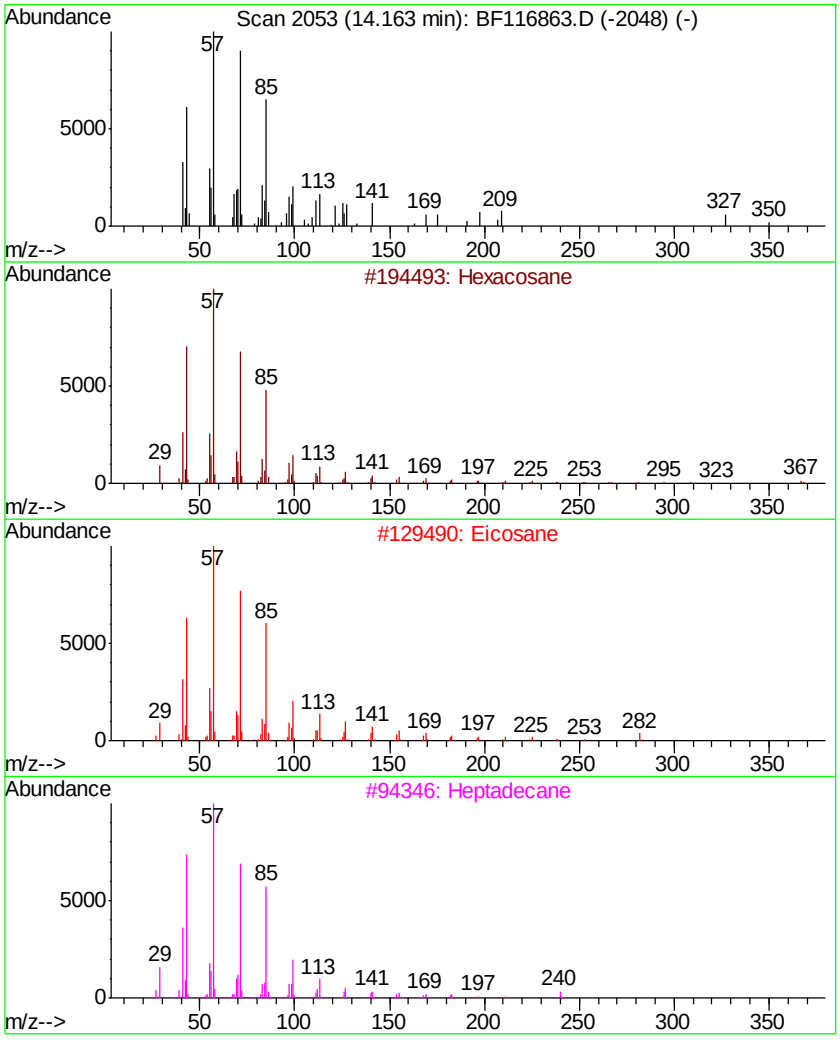
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

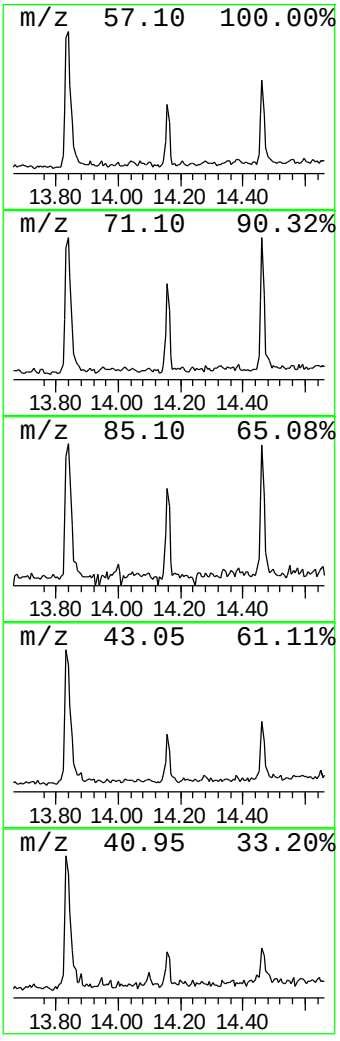
****

Peak Number 6 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.16	2.16 ng	45599	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	83
2	Eicosane	282	C20H42	000112-95-8	83
3	Heptadecane	240	C17H36	000629-78-7	83
4	Tetratetracontane	619	C44H90	007098-22-8	83
5	Hexadecane	226	C16H34	000544-76-3	80





Library Search Compound Report

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Operator : HP/JU
Sample : K4650-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

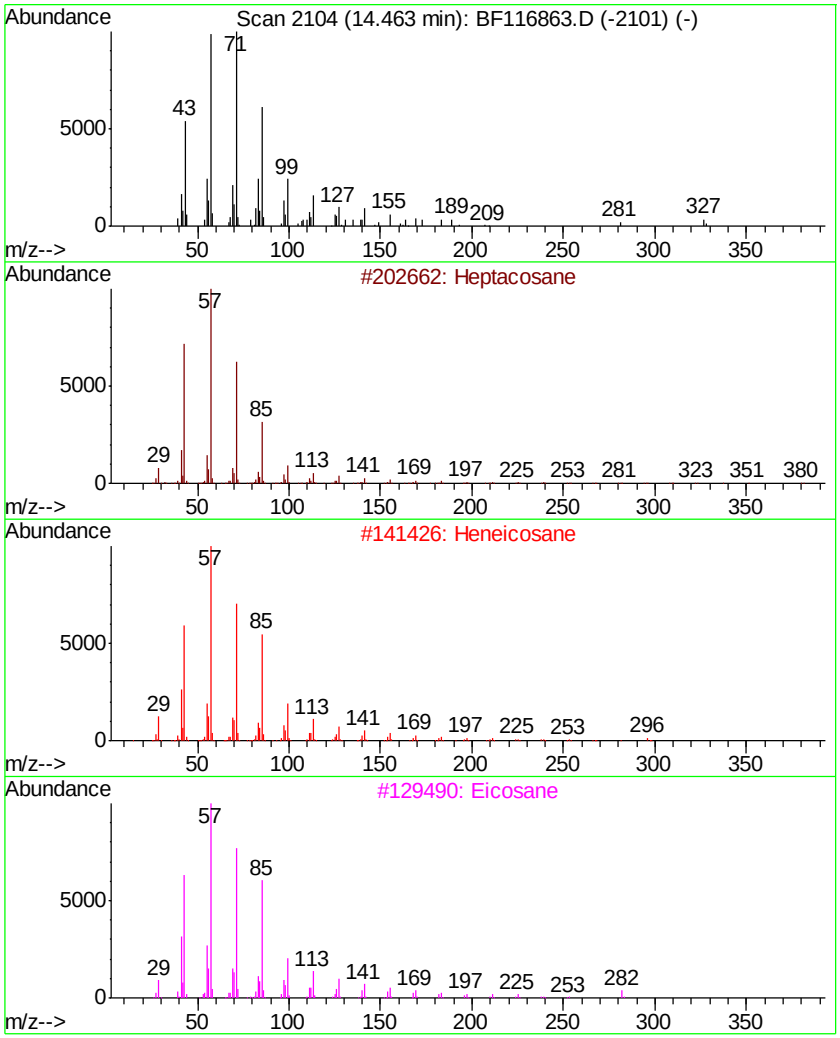
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

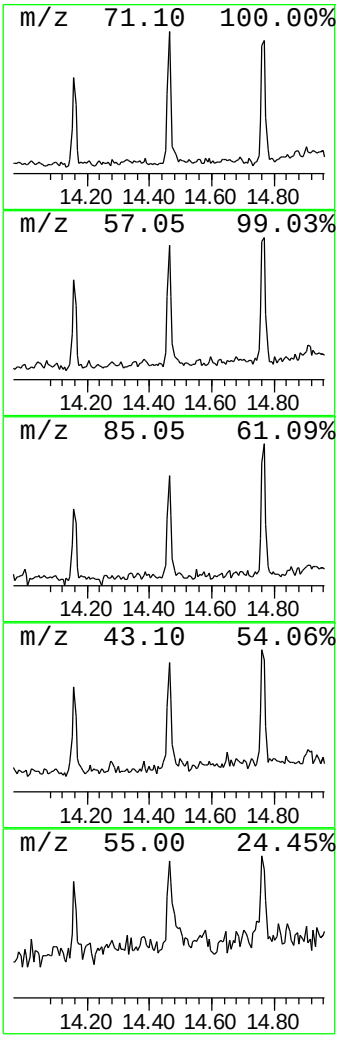
****

Peak Number 7 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.46	2.79 ng	58961	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Eicosane	282	C20H42	000112-95-8	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Triacontane	422	C30H62	000638-68-6	87





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

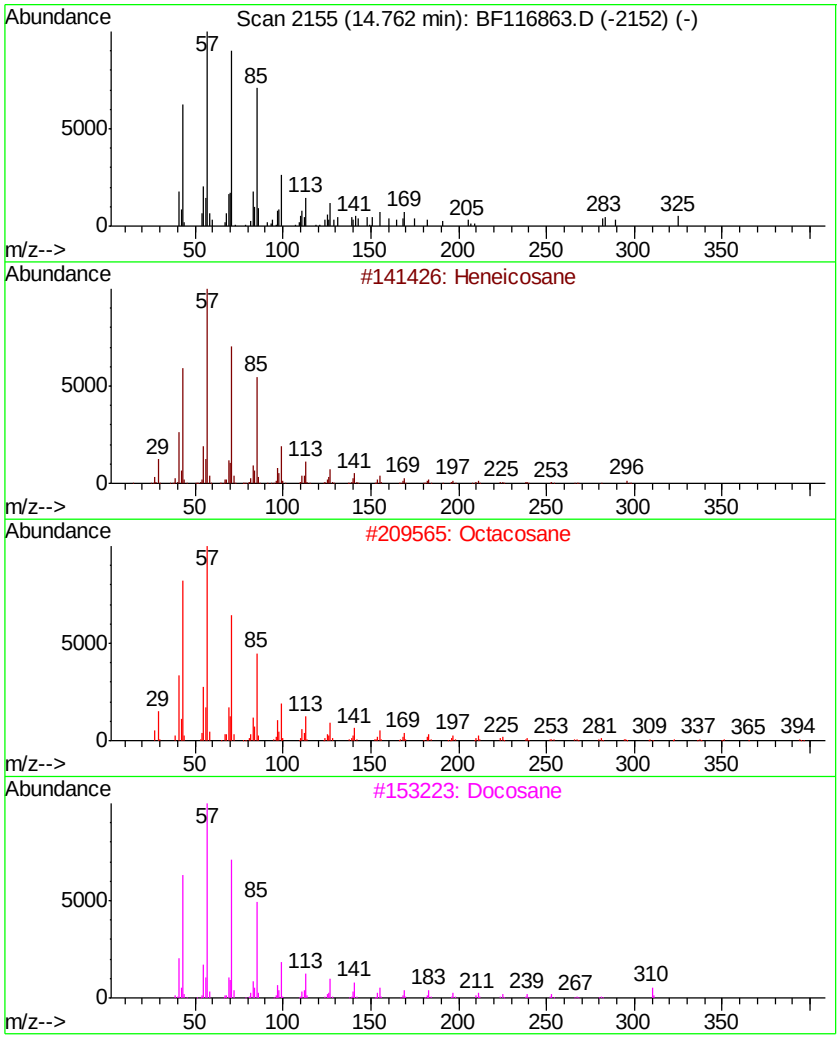
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

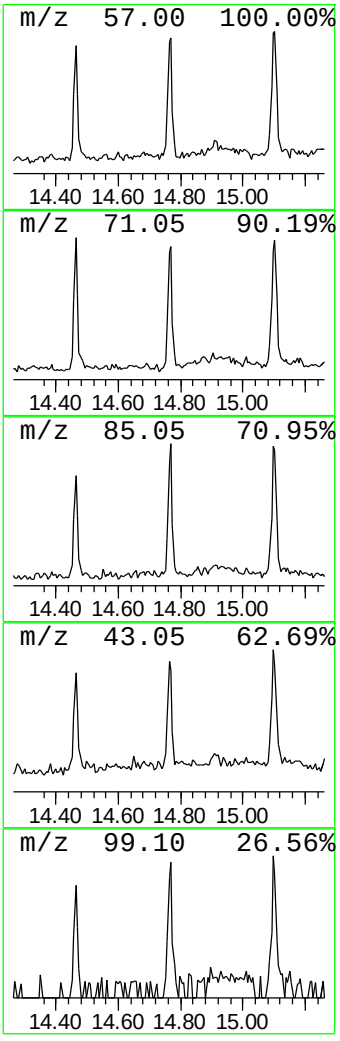
****

Peak Number 8 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.76	2.71 ng	72034	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	87
2	Octacosane	394	C28H58	000630-02-4	86
3	Docosane	310	C22H46	000629-97-0	86
4	Heptadecane	240	C17H36	000629-78-7	86
5	Eicosane	282	C20H42	000112-95-8	81





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Misc :
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Instrument : BNA_F
ClientSampleId : TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

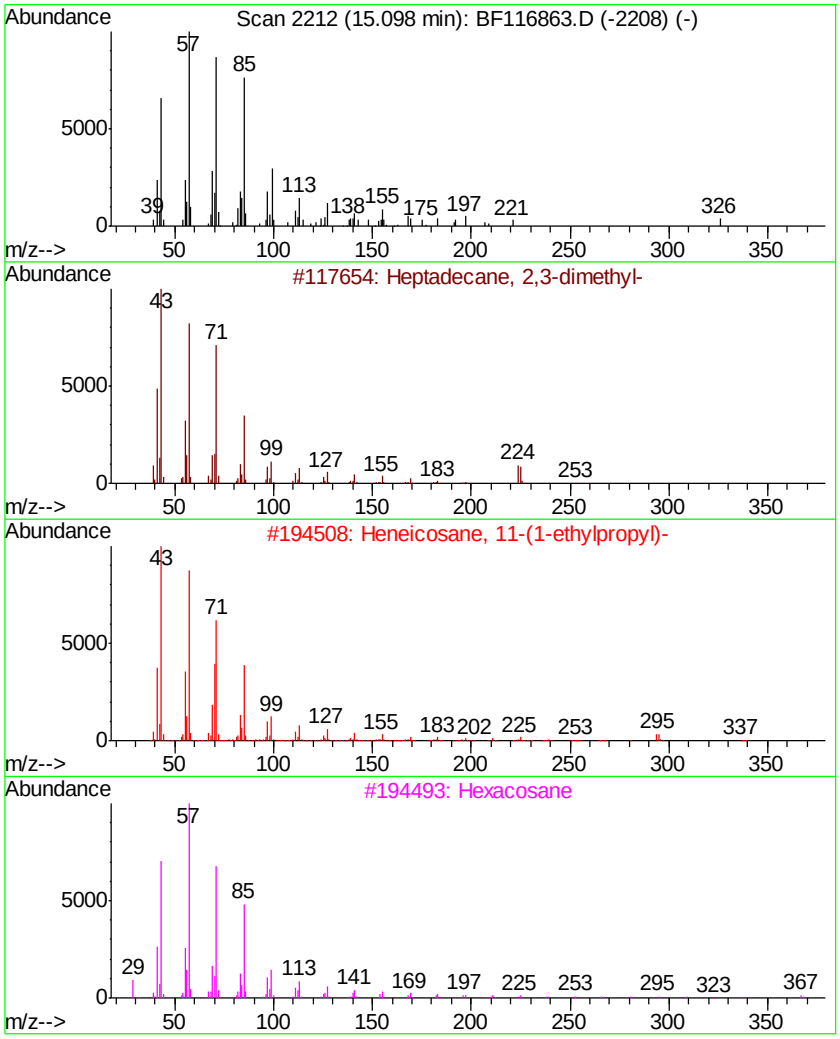
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

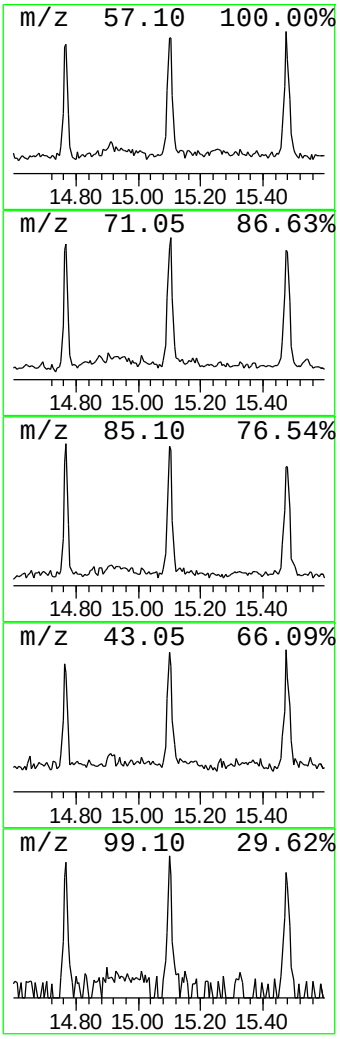
****

Peak Number 9 Heptadecane, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.10	3.31 ng	87814	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,3-dimethyl-	268	C19H40	061868-03-9	91
2	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	90
5	Heptacosane	380	C27H56	000593-49-7	86





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Sample : K4650-11
Misc :
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Instrument : BNA_F
ClientSampleId : TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

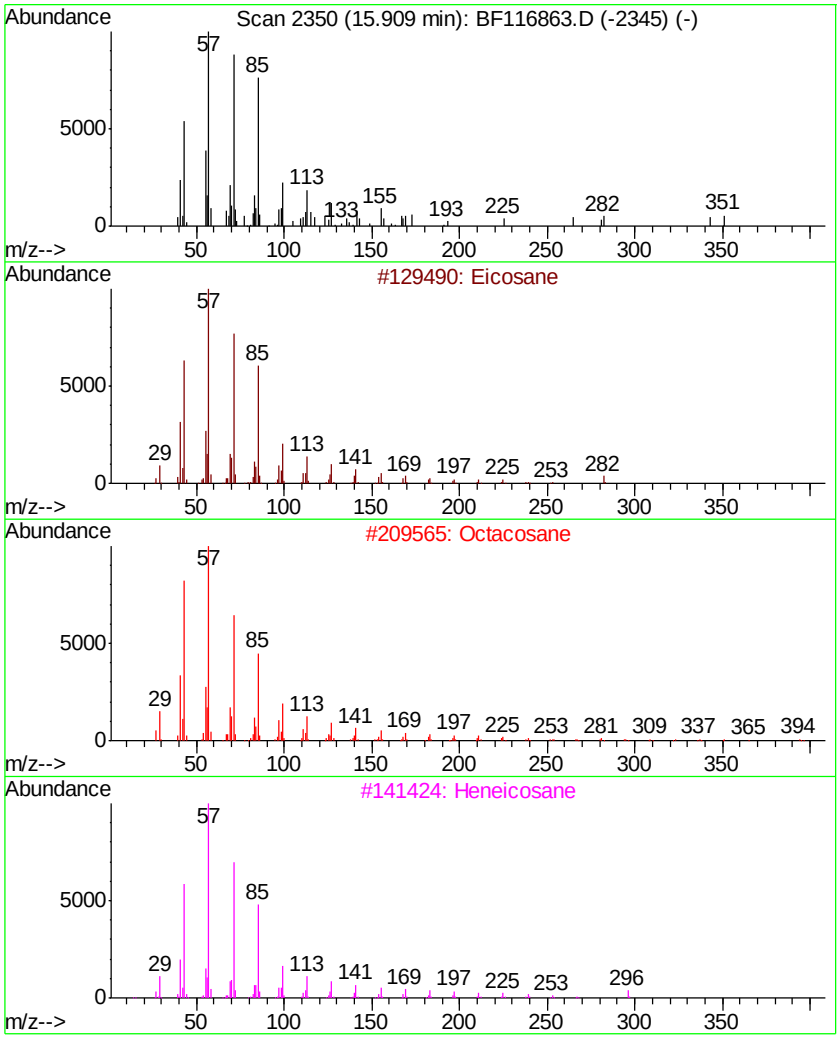
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

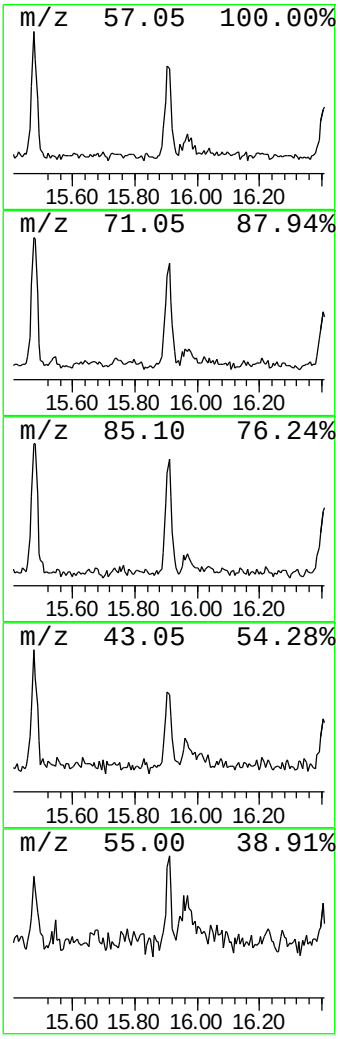
****

Peak Number 10 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.91	2.78 ng	73702	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	98
2	Octacosane	394	C28H58	000630-02-4	87
3	Heneicosane	296	C21H44	000629-94-7	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	86





Tentatively Identified Compound (LSC) summary

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Data File : BF116863.D
Acq On : 6 Sep 2019 15:53
Operator : HP/JU
Sample : K4650-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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...	2.11	15.0	ng	334255	1	6.85	444354	20.0
unknown6.62	6.62	70.0	ng	1555140	1	6.85	444354	20.0
n-Hexadecanoic acid	11.89	4.2	ng	129507	4	11.36	614287	20.0
n-Nonadecanol-1	13.83	11.8	ng	249206	5	14.00	423001	20.0
Hexacosane	14.16	2.2	ng	45599	5	14.00	423001	20.0
Heptacosane	14.46	2.8	ng	58961	5	14.00	423001	20.0
Heneicosane	14.76	2.7	ng	72034	6	15.46	531010	20.0
Heptadecane, 2,3-...	15.10	3.3	ng	87814	6	15.46	531010	20.0
Eicosane	15.91	2.8	ng	73702	6	15.46	531010	20.0