LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091218\
Data File : BF108951.D
Acq On : 12 Sep 2018 15:40
Operator : JU/SJ
Sample : PB112774BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

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-BF090518.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	4.954	439	445	454	rVB	106886	146764	3.28%	0.393%
2	5.360	508	514	517	rBV	3278396	3491388	78.08%	9.338%
3	6.372	680	686	689	rBV	3350636	3635047	81.29%	9.723%
4	6.507	704	709	712	rBV	3740213	3618200	80.91%	9.678%
5	6.737	744	748	751	rBV	1259923	1026850	22.96%	2.747%
6	6.895	770	775	778	rBV	3116677	2902784	64.91%	7.764%
7	7.295	837	843	846	rBV	2355880	2381978	53.27%	6.371%
8	8.019	961	966	969	rBV	1342303	1314195	29.39%	3.515%
9	9.095	1143	1149	1152	rBV	4636737	4328961	96.81%	11.579%
10	9.766	1257	1263	1267	rBV2	1764665	1541397	34.47%	4.123%
11	10.554	1392	1397	1400	rBV	2565445	2655676	59.39%	7.103%
12	11.242	1510	1514	1518	rBV	1901971	1626402	36.37%	4.350%
13	12.830	1779	1784	1787	rBV	4484252	4471736	100.00%	11.961%
14	13.871	1956	1961	1964	rBV	1634829	1598768	35.75%	4.276%
15	14.360	2041	2044	2050	rVB	66456	65382	1.46%	0.175%
16	14.654	2082	2094	2102	rBV	154533	182247	4.08%	0.487%
17	14.971	2143	2148	2153	rBV	207757	226187	5.06%	0.605%
18	15.277	2195	2200	2205	rBV	1047091	1255228	28.07%	3.357%
19	15.330	2205	2209	2216	rVB	254560	327039	7.31%	0.875%
20	15.736	2273	2278	2287	rVB	204656	304969	6.82%	0.816%
21	16.207	2352	2358	2366	rBV	120259	210361	4.70%	0.563%
22	16.759	2447	2452	2459	rVB2	41676	75879	1.70%	0.203%

Sum of corrected areas: 37387438

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091218\
Data File : BF108951.D
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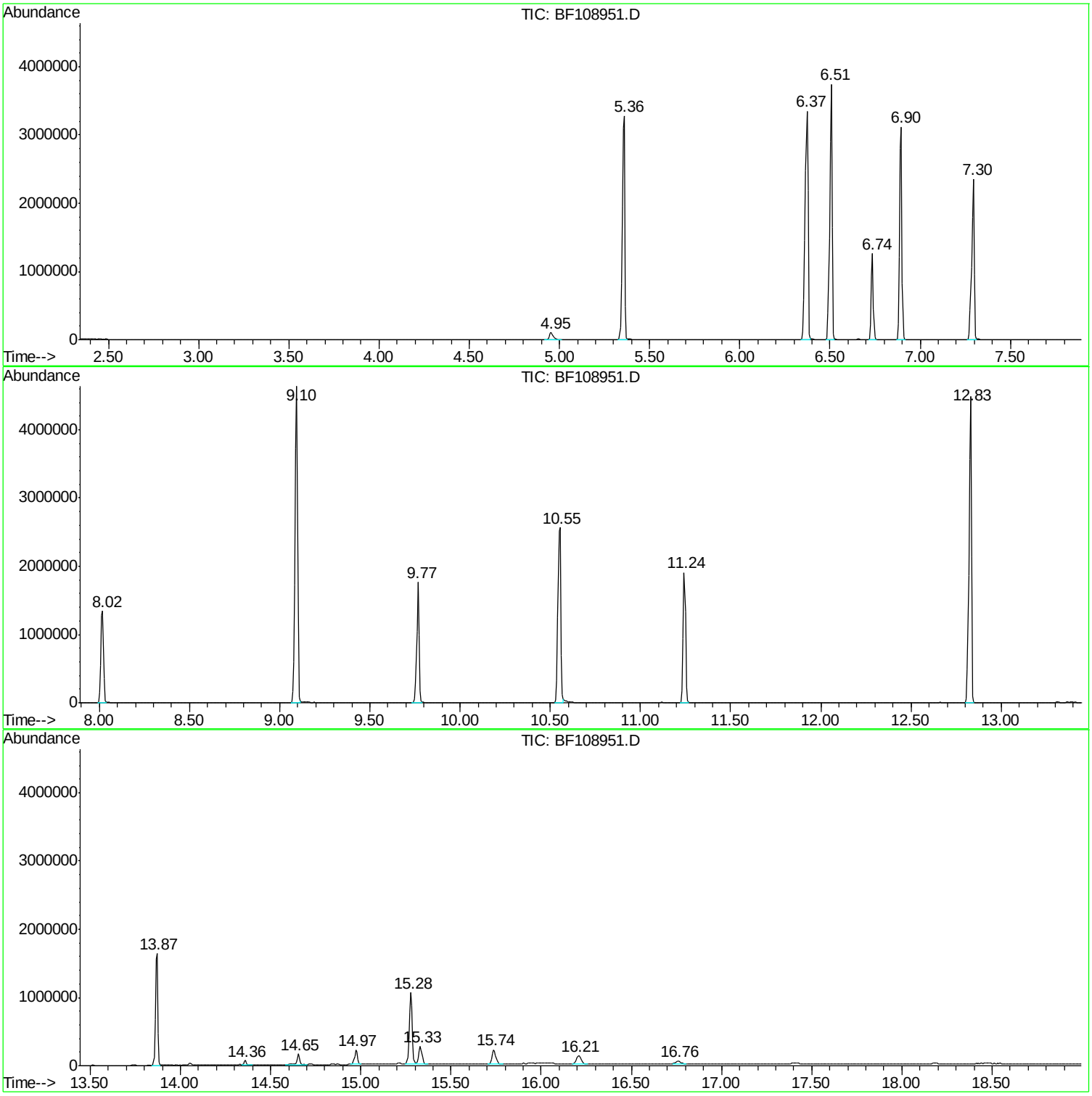
Sample : PB112774BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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\BF091218\
Data File : BF108951.D
Acq On : 12 Sep 2018 15:40
Operator : JU/SJ
Sample : PB112774BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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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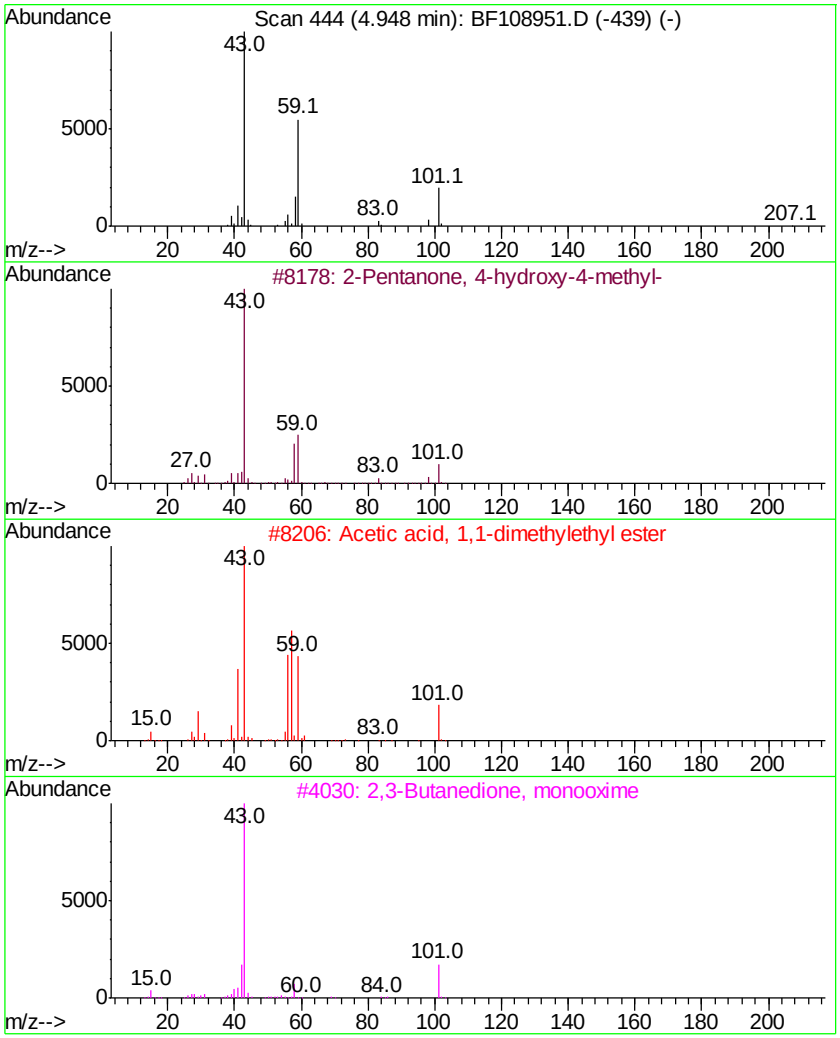
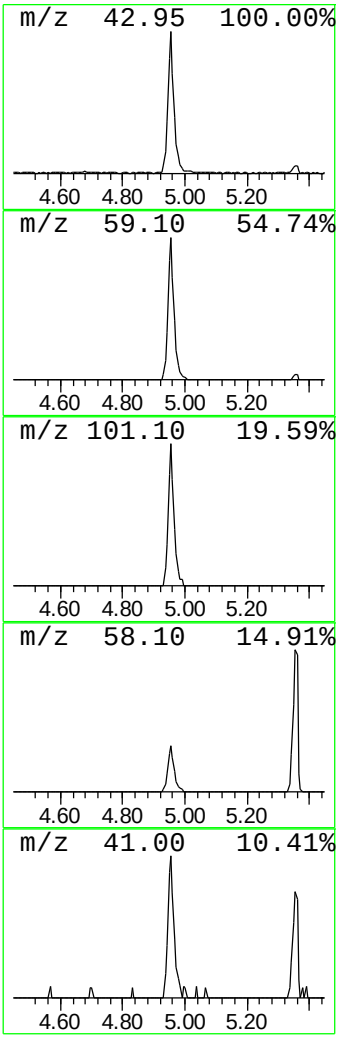
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.95	2.86 ng	146764	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
4	3-Hexanol	102	C6H14O	000623-37-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091218\
Data File : BF108951.D
Acq On : 12 Sep 2018 15:40
Operator : JU/SJ
Sample : PB112774BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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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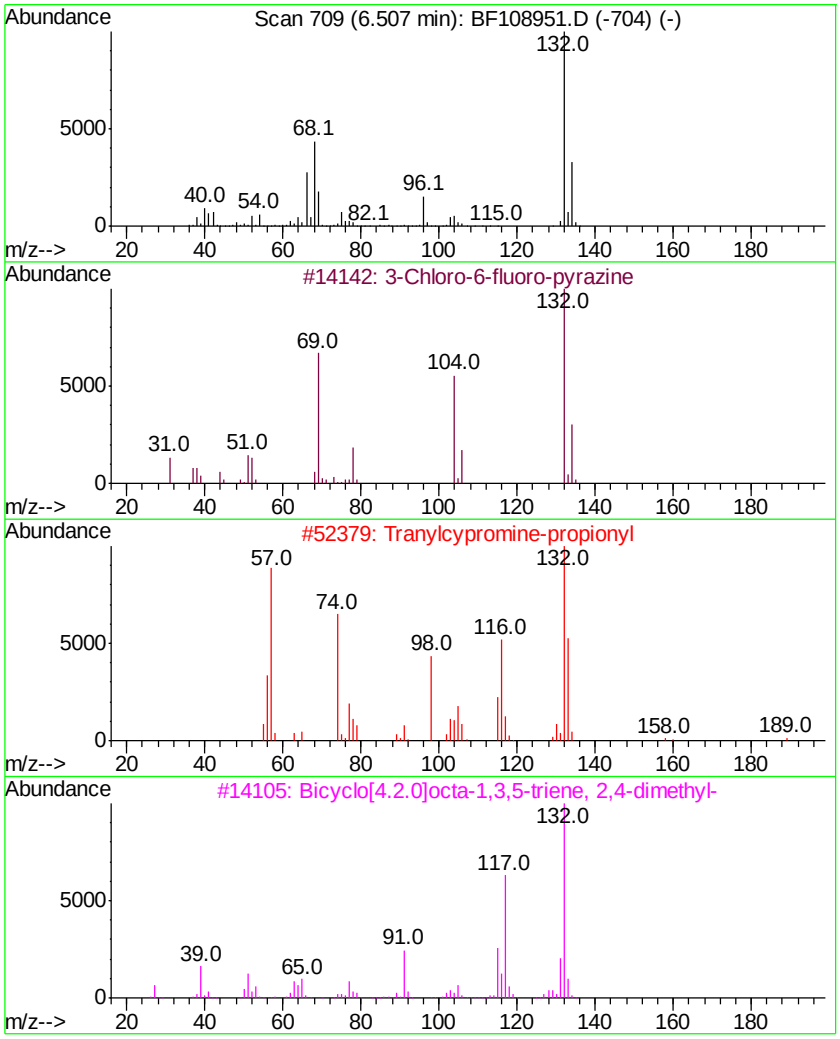
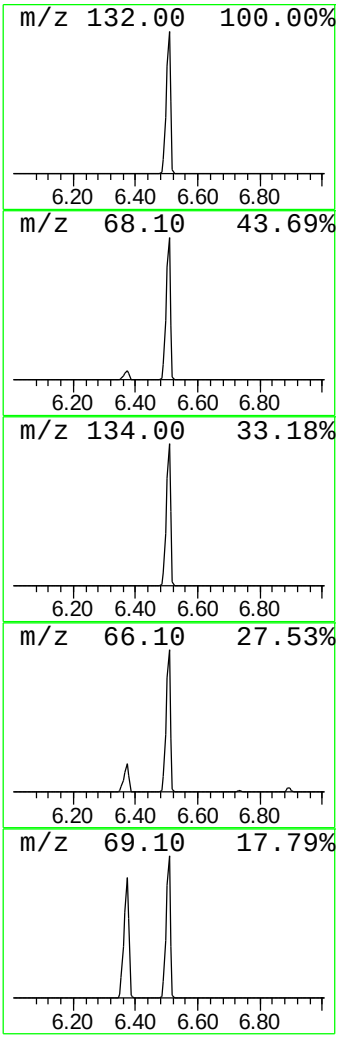
Peak Number 2 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	70.47 ng	3618200	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091218\
Data File : BF108951.D
Acq On : 12 Sep 2018 15:40
Operator : JU/SJ
Sample : PB112774BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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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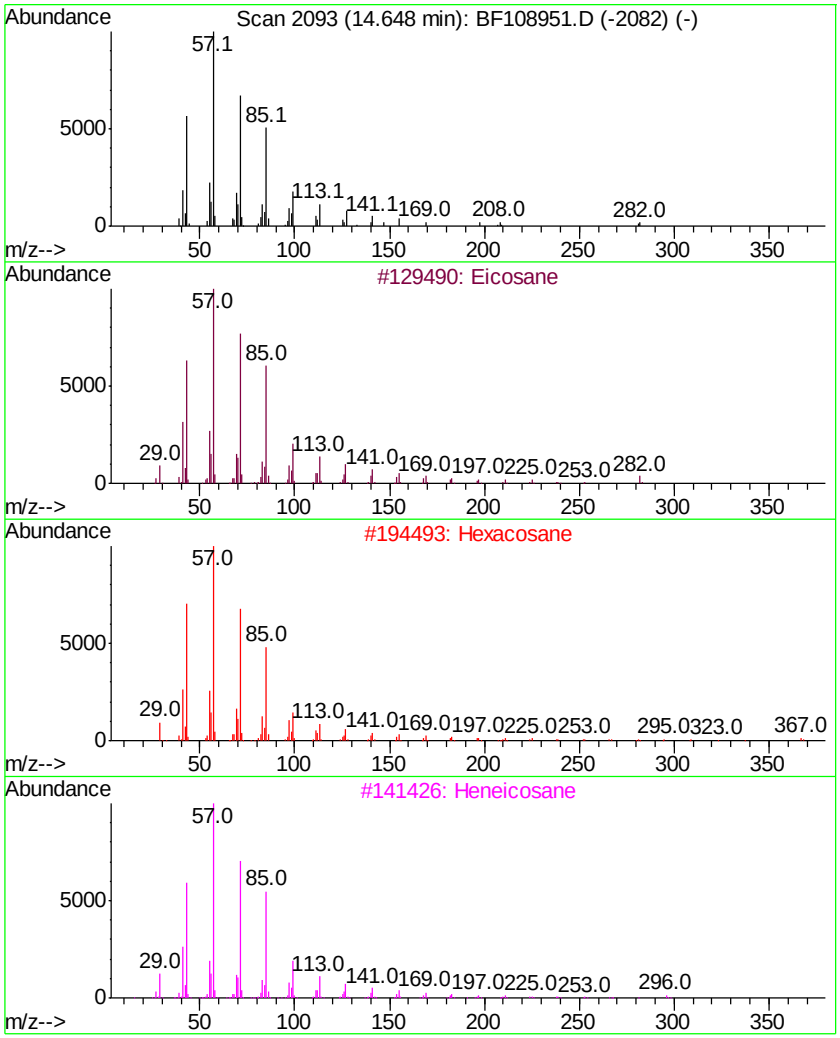
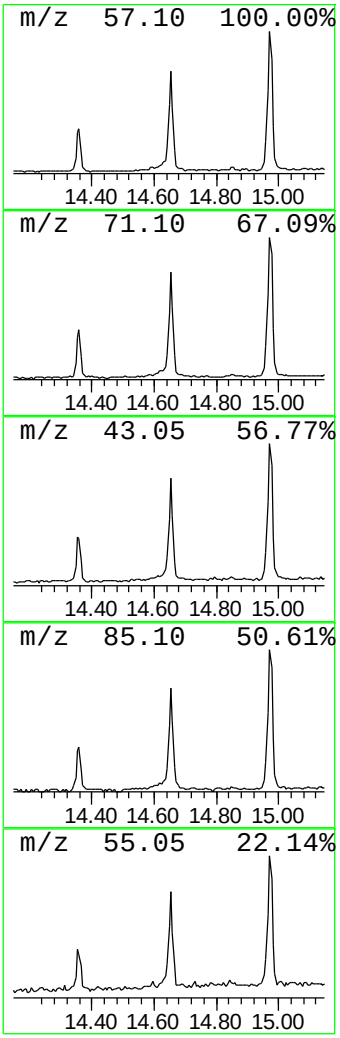
Peak Number 4 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	2.90 ng	182247	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Heptadecane	240	C17H36	000629-78-7	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091218\
Data File : BF108951.D
Acq On : 12 Sep 2018 15:40
Operator : JU/SJ
Sample : PB112774BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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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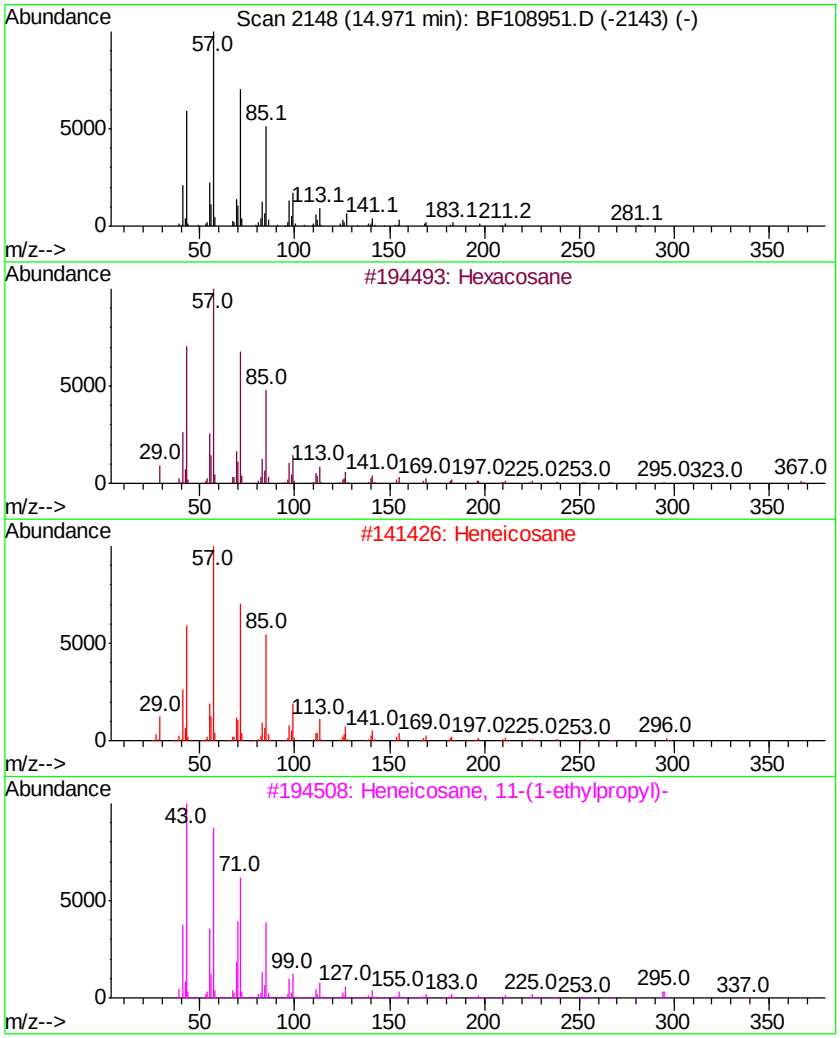
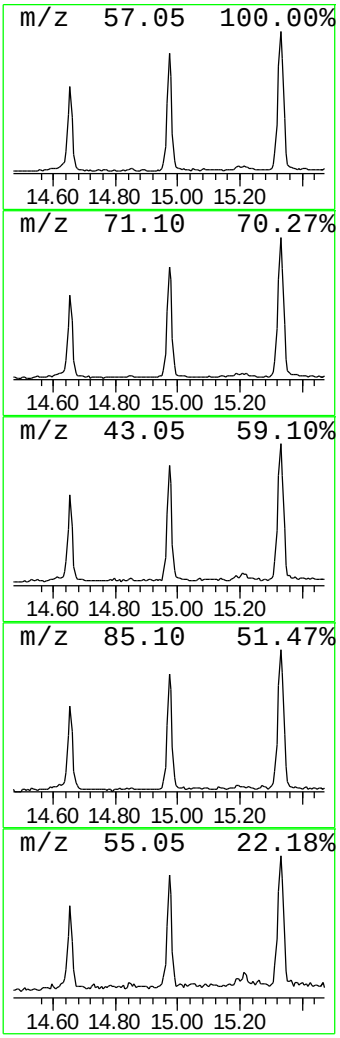
Peak Number 5 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	3.60 ng	226187	Perylene-d12	15.28

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	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
4	Octadecane	254	C18H38	000593-45-3	87
5	Tetratetracontane	619	C44H90	007098-22-8	87





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Data File : BF108951.D
Acq On : 12 Sep 2018 15:40
Operator : JU/SJ
Sample : PB112774BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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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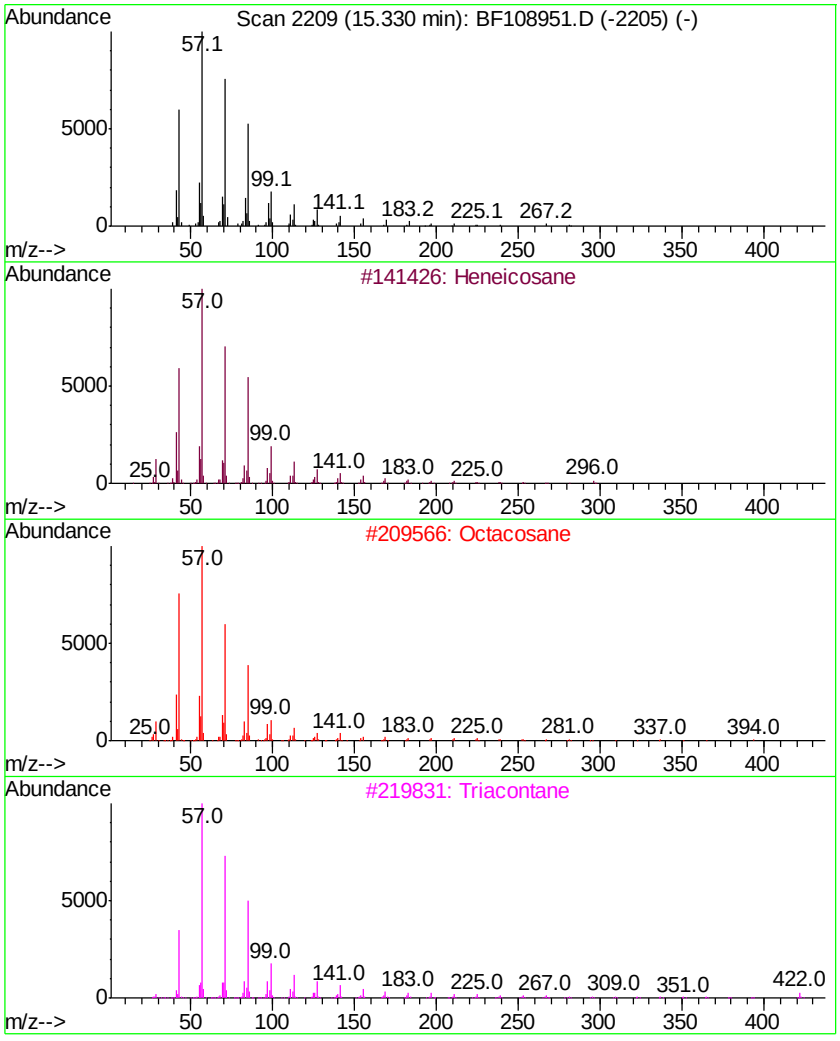
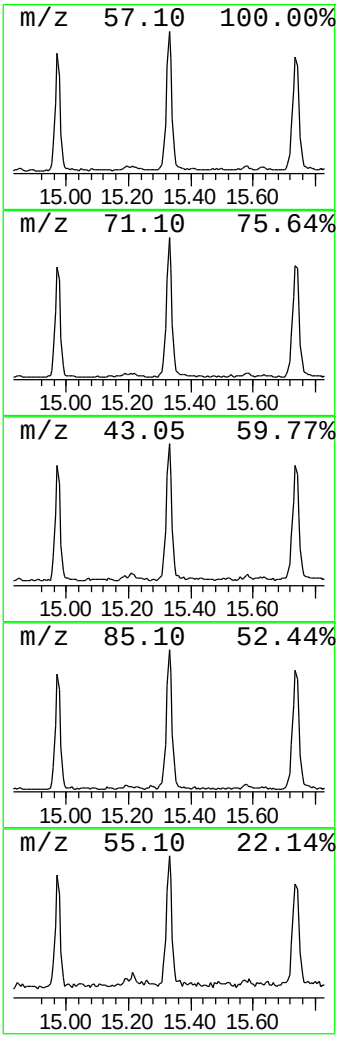
Peak Number 6 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.33	5.21 ng	327039	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Eicosane, 2-methyl-	296	C21H44	001560-84-5	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091218\
Data File : BF108951.D
Acq On : 12 Sep 2018 15:40
Operator : JU/SJ
Sample : PB112774BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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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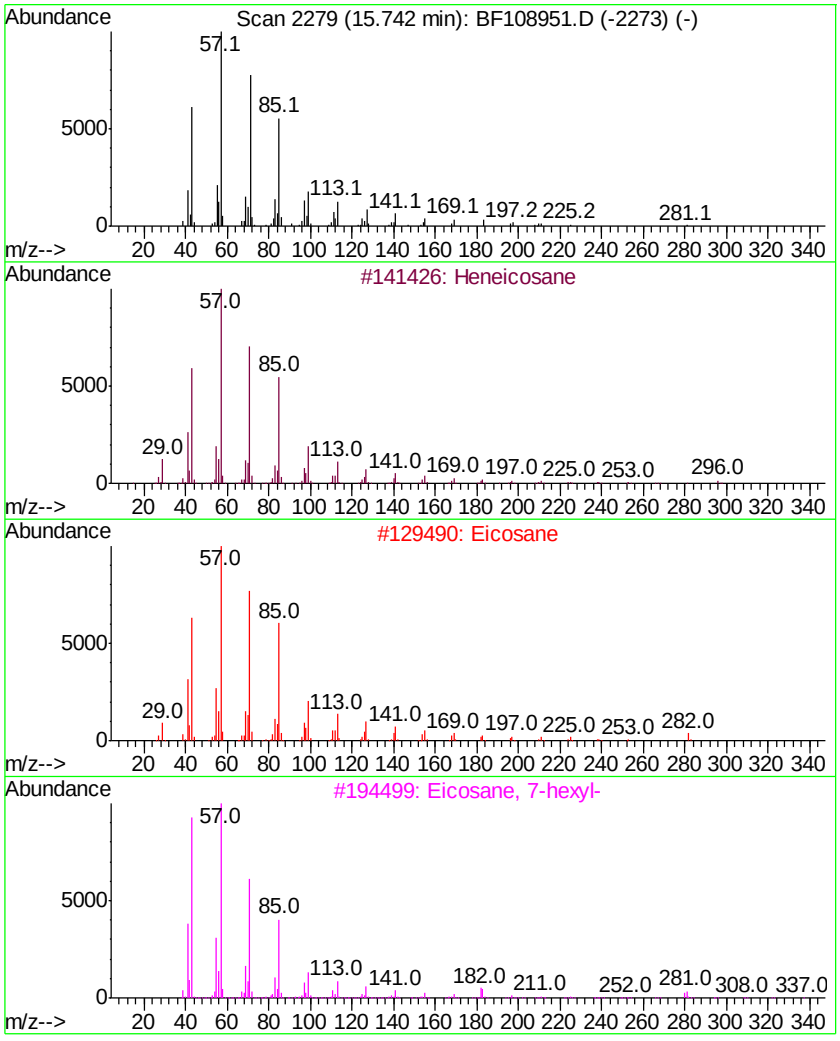
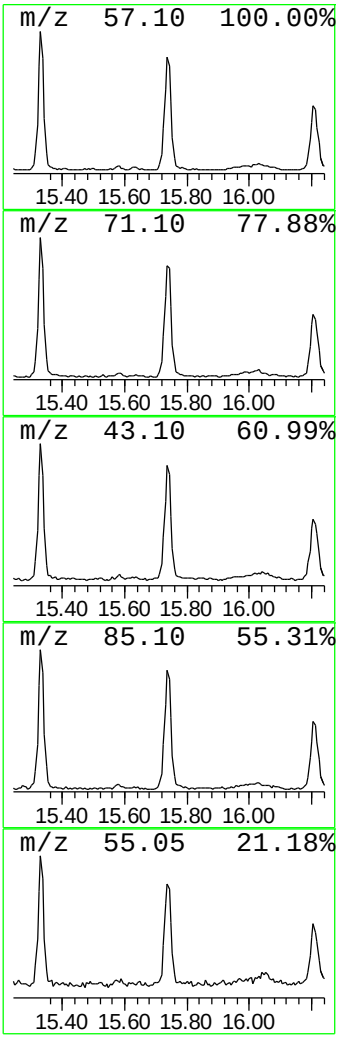
Peak Number 7 Eicosane, 7-hexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	4.86 ng	304969	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
4	Octadecane, 2-methyl-	268	C19H40	001560-88-9	90
5	2-Bromotetradecane	276	C14H29Br	074036-95-6	90





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Sample : PB112774BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

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TIC Library : C:\DATABASE\NIST11.L
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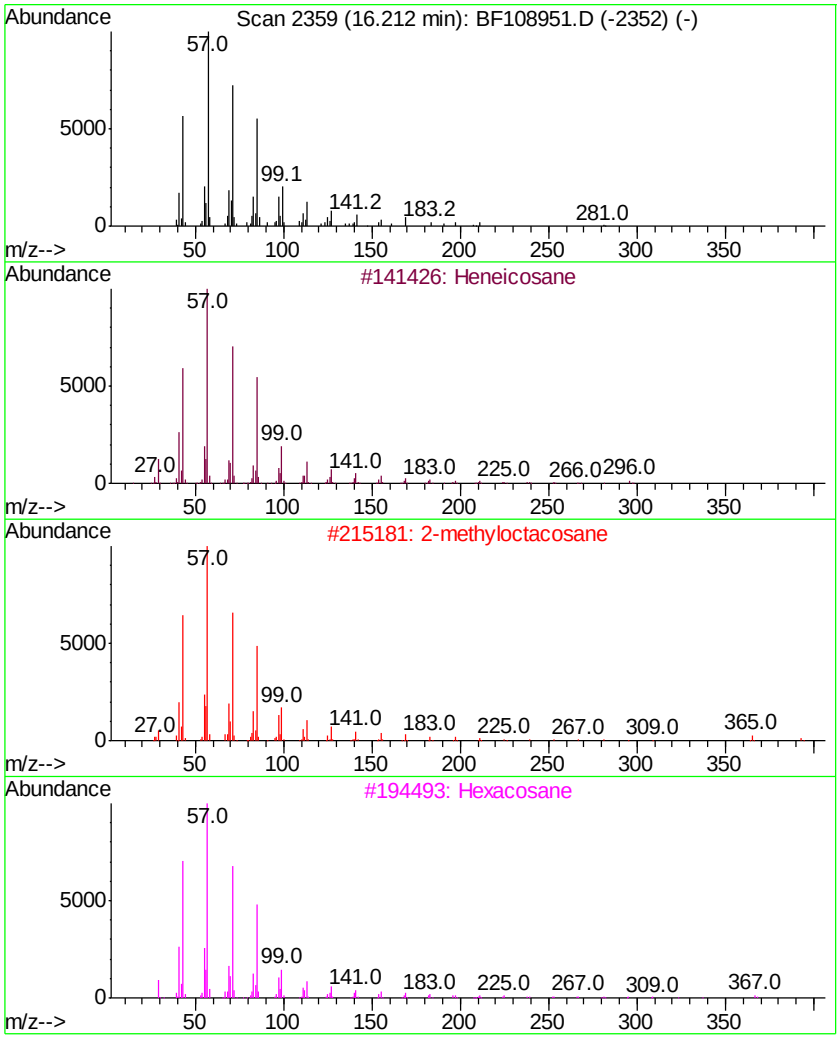
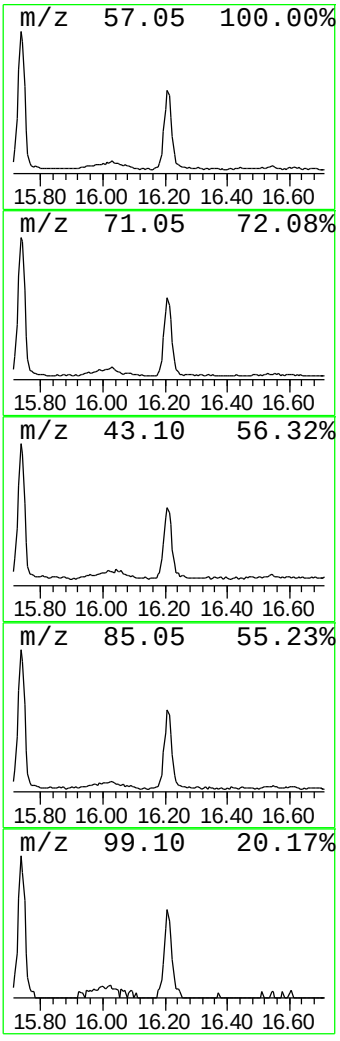
Peak Number 8 2-methyloctacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.21	3.35 ng	210361	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Hexacosane	366	C26H54	000630-01-3	90
4	Eicosane	282	C20H42	000112-95-8	90
5	Heptadecane	240	C17H36	000629-78-7	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091218\
Data File : BF108951.D
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Operator : JU/SJ
Sample : PB112774BL
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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...	4.95	2.9	ng	146764	1	6.74	1026850	20.0
unknown6.51	6.51	70.5	ng	3618200	1	6.74	1026850	20.0
Eicosane	14.65	2.9	ng	182247	6	15.28	1255230	20.0
Hexacosane	14.97	3.6	ng	226187	6	15.28	1255230	20.0
Heneicosane	15.33	5.2	ng	327039	6	15.28	1255230	20.0
Eicosane, 7-hexyl-	15.74	4.9	ng	304969	6	15.28	1255230	20.0
2-methyloctacosane	16.21	3.4	ng	210361	6	15.28	1255230	20.0