LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP100419\
Data File : BP000528.D
Acq On : 04 Oct 2019 23:37
Operator : JU
Sample : K5154-19
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : MW-104D

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_P\METHODS\8270-BP100119.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	5.393	558	562	566	rBV	4648439	4285582	52.40%	7.220%
2	6.410	730	735	753	rBV	3473068	3581591	43.79%	6.034%
3	6.540	753	757	760	rBV	6376184	5996386	73.31%	10.102%
4	6.769	792	796	799	rBV	1957375	1642045	20.08%	2.766%
5	6.922	818	822	826	rBV	5278122	4690765	57.35%	7.902%
6	7.328	886	891	894	rBV	4295810	3752036	45.87%	6.321%
7	8.051	1010	1014	1017	rBV	2508313	2085764	25.50%	3.514%
8	8.445	1076	1081	1093	rBV	423580	446334	5.46%	0.752%
9	9.134	1193	1198	1201	rBV	8199906	7408305	90.58%	12.480%
10	9.522	1261	1264	1268	rBV	753189	641164	7.84%	1.080%
11	9.810	1310	1313	1317	rVB	3001611	2464253	30.13%	4.151%
12	10.610	1444	1449	1452	rBV	5212118	4862286	59.45%	8.191%
13	11.310	1564	1568	1571	rBV	2713166	2478191	30.30%	4.175%
14	11.375	1574	1579	1583	rVB3	123155	118704	1.45%	0.200%
15	11.851	1656	1660	1674	rBV2	544168	654767	8.01%	1.103%
16	12.645	1792	1795	1802	rBV	158871	177555	2.17%	0.299%
17	12.916	1836	1841	1844	rBV	8601610	8179084	100.00%	13.779%
18	13.827	1992	1996	2013	rBV3	574922	903353	11.04%	1.522%
19	13.974	2017	2021	2025	rBV	2465461	2270104	27.75%	3.824%
20	14.157	2048	2052	2061	rBV	174412	184366	2.25%	0.311%
21	14.463	2101	2104	2111	rVB	158145	144651	1.77%	0.244%
22	14.774	2153	2157	2162	rVB	212593	210337	2.57%	0.354%
23	15.116	2211	2215	2220	rVB	232741	251731	3.08%	0.424%
24	15.457	2267	2273	2277	rBV	1061266	1265299	15.47%	2.132%
25	15.498	2277	2280	2288	rVB	207020	283912	3.47%	0.478%
26	15.939	2351	2355	2361	rBV	148751	224790	2.75%	0.379%
27	16.451	2438	2442	2453	rVB2	82779	157323	1.92%	0.265%

Sum of corrected areas: 59360678

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Misc :
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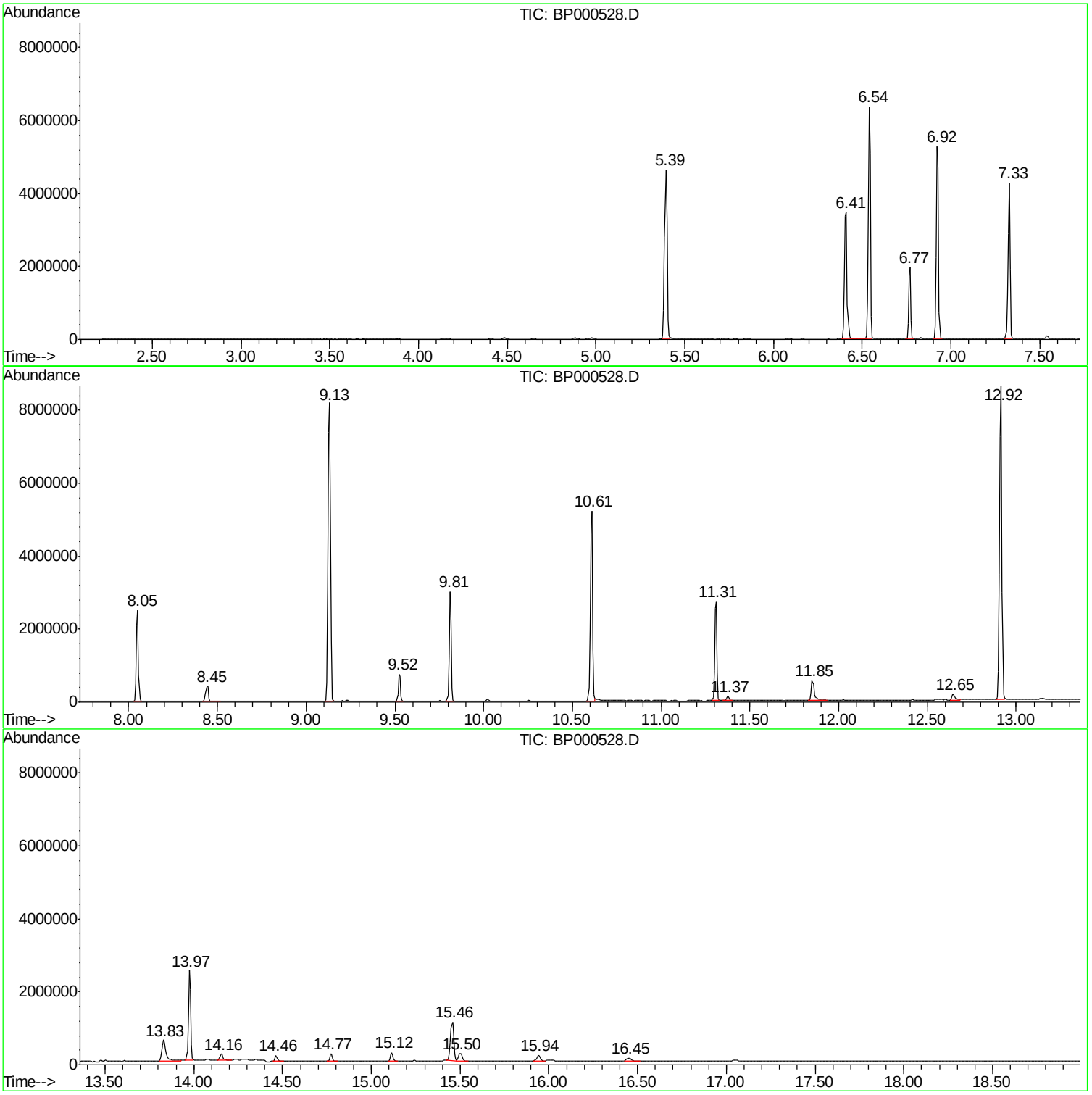
Instrument :
BNA_P
ClientSampleId :
MW-104D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.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

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

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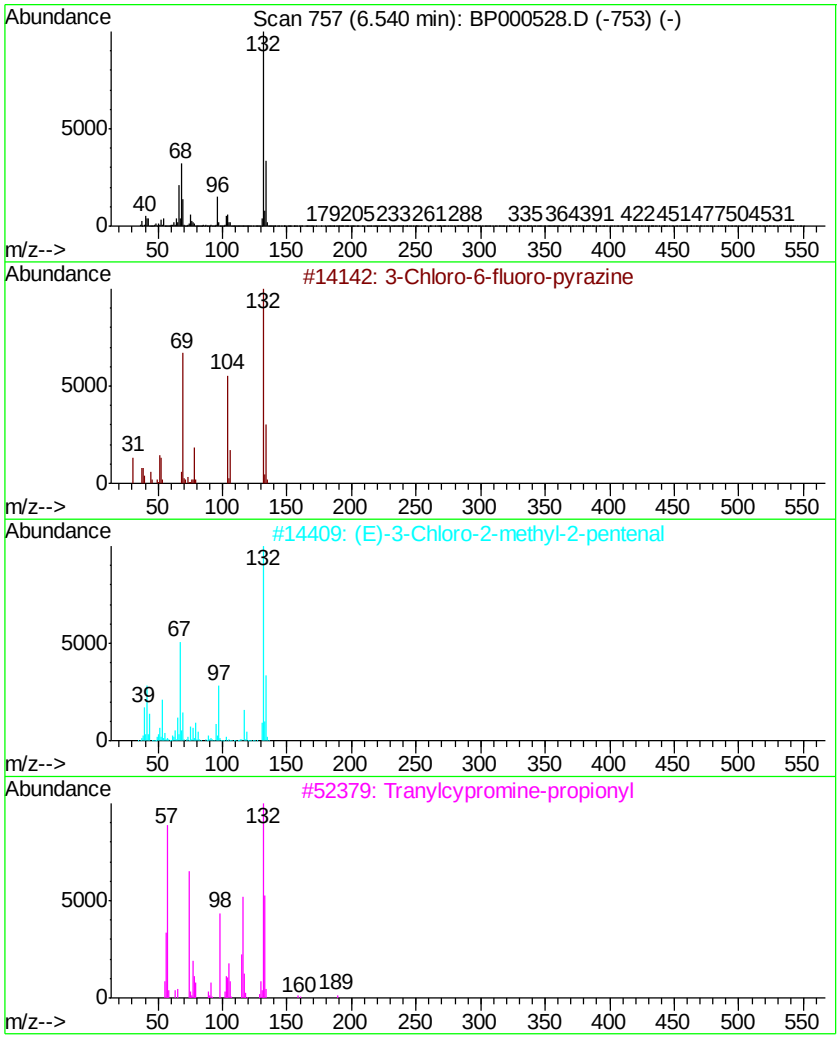
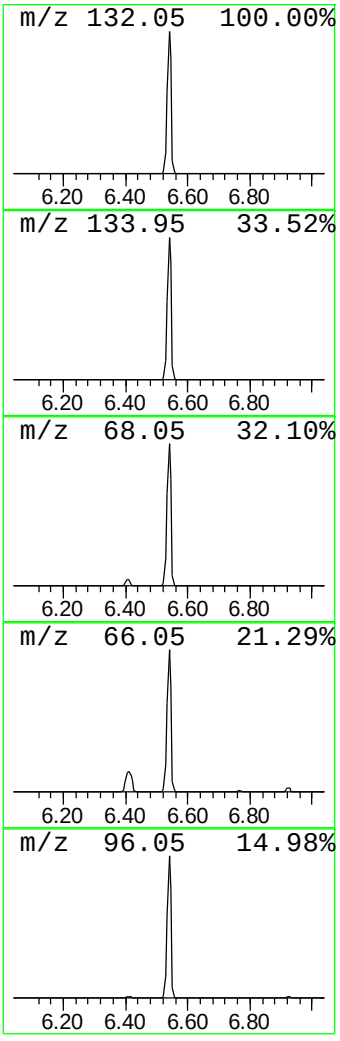
Peak Number 1 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	73.04 ng	5996390	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Library Search Compound Report

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Operator : JU
Sample : K5154-19
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : MW-104D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.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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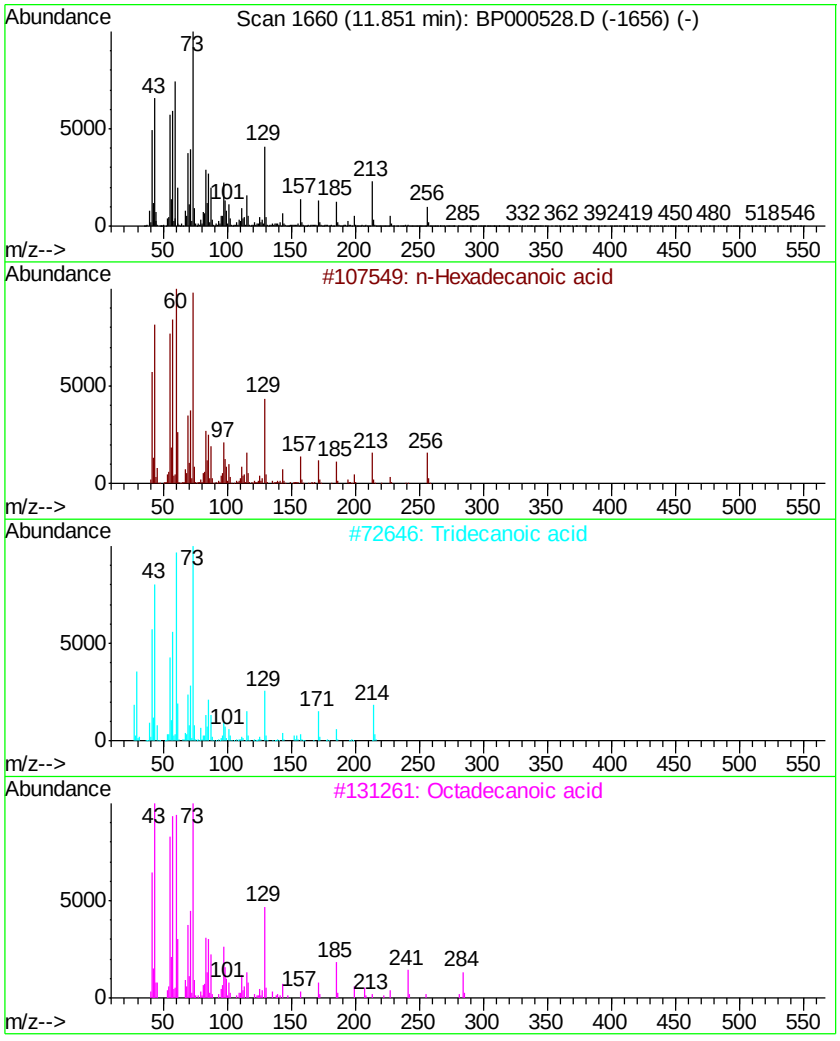
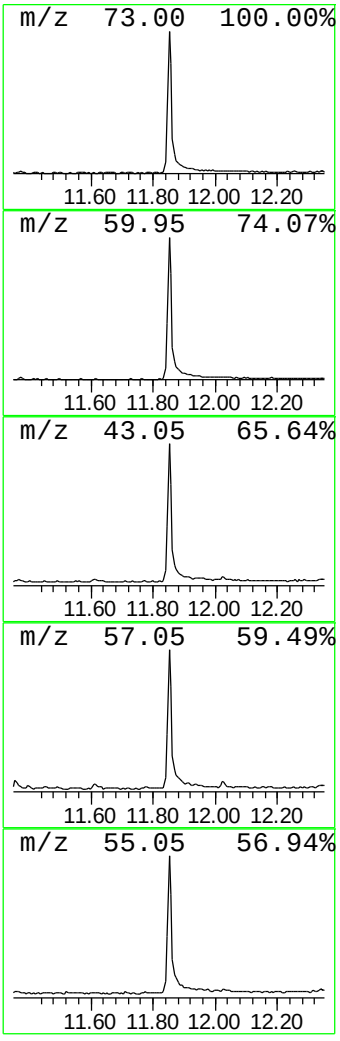
Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	5.28 ng	654767	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Octadecanoic acid	284	C18H36O2	000057-11-4	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	80





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Acq On : 04 Oct 2019 23:37
Operator : JU
Sample : K5154-19
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : MW-104D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.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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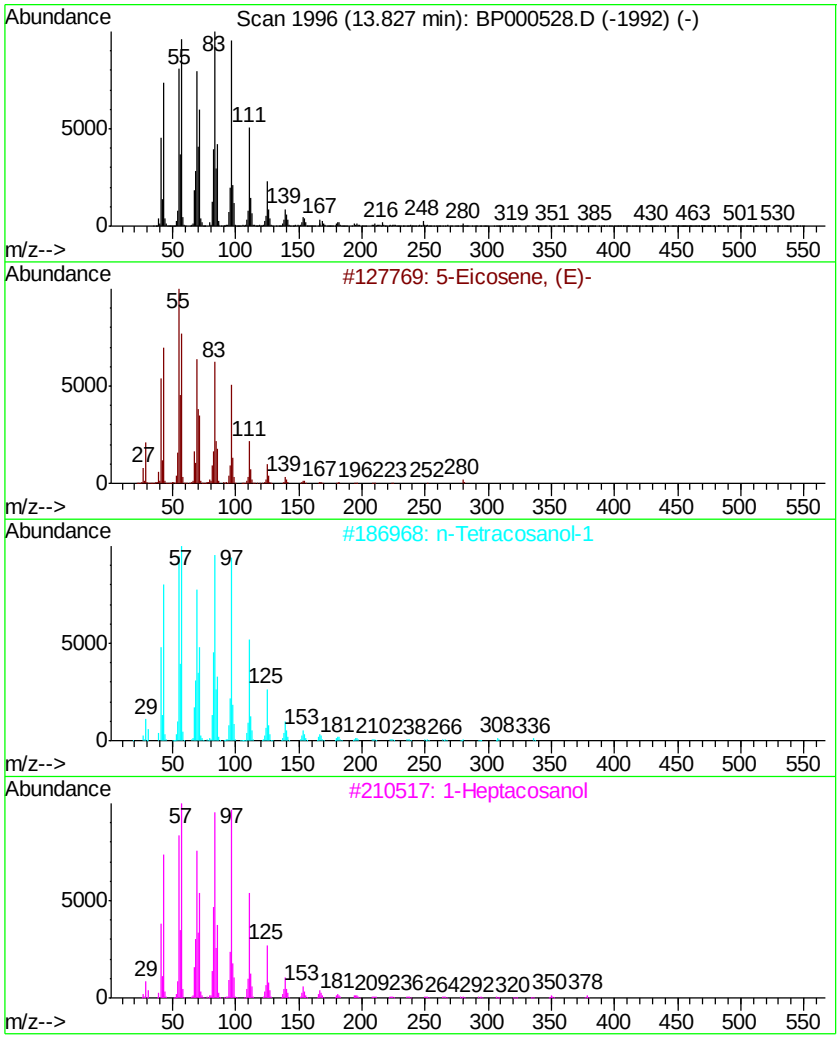
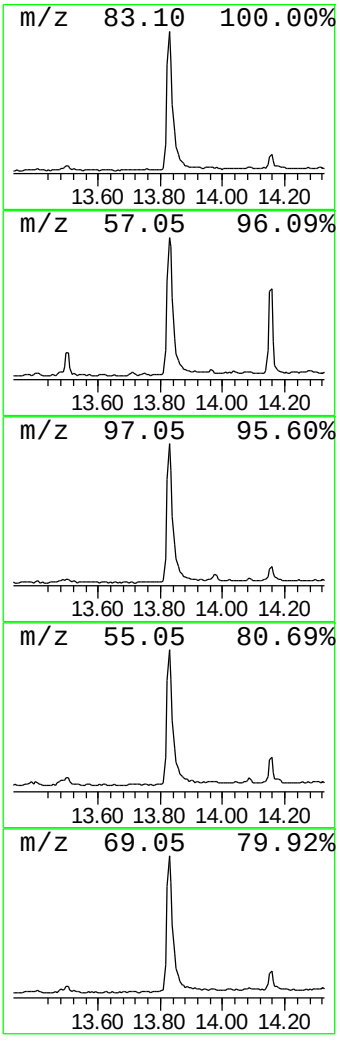
Peak Number 4 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	7.96 ng	903353	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	1-Heptacosanol	396	C27H56O	002004-39-9	95
4	1-Heneicosanol	312	C21H44O	015594-90-8	94
5	Behenic alcohol	326	C22H46O	000661-19-8	94





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ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : MW-104D

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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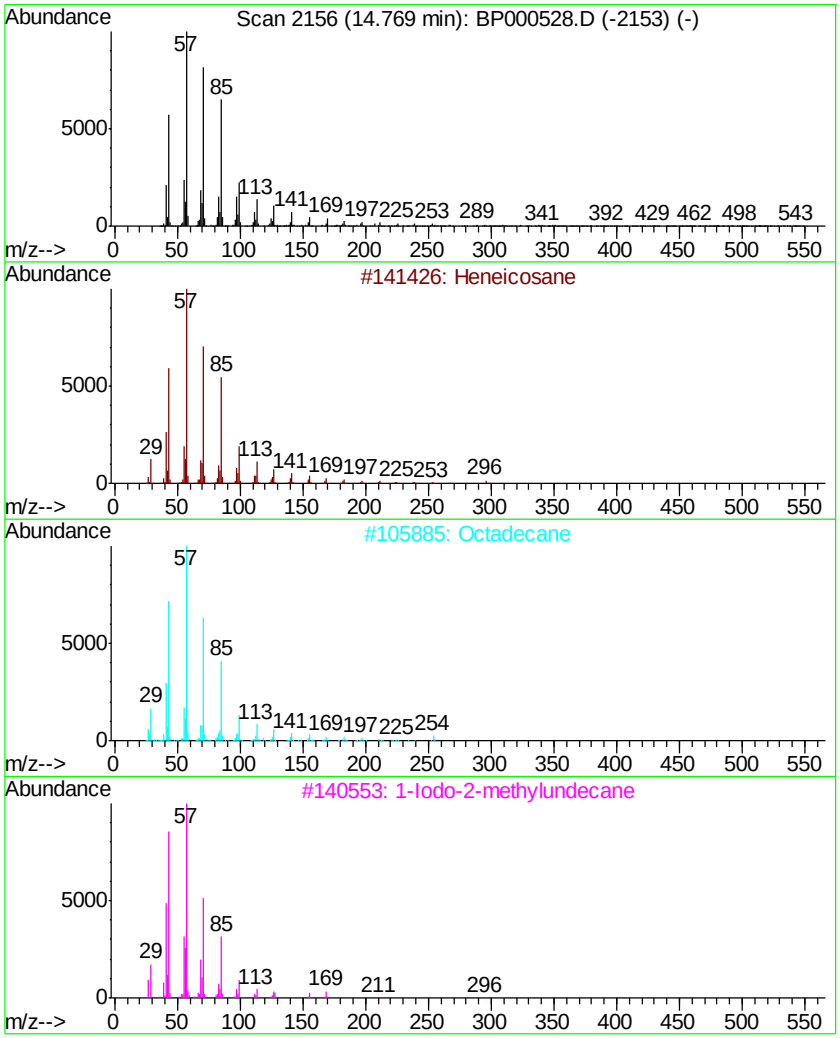
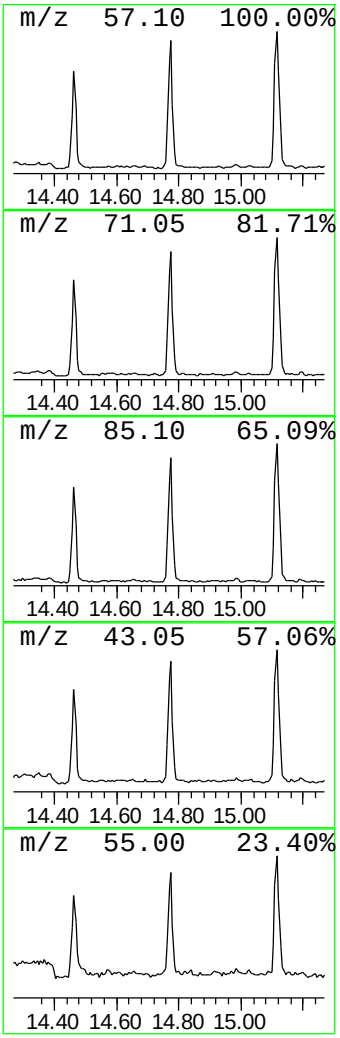
Peak Number 5 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.77	3.32 ng	210337	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	96
2	Octadecane	254	C18H38	000593-45-3	95
3	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	94
4	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	93
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





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Instrument : BNA_P
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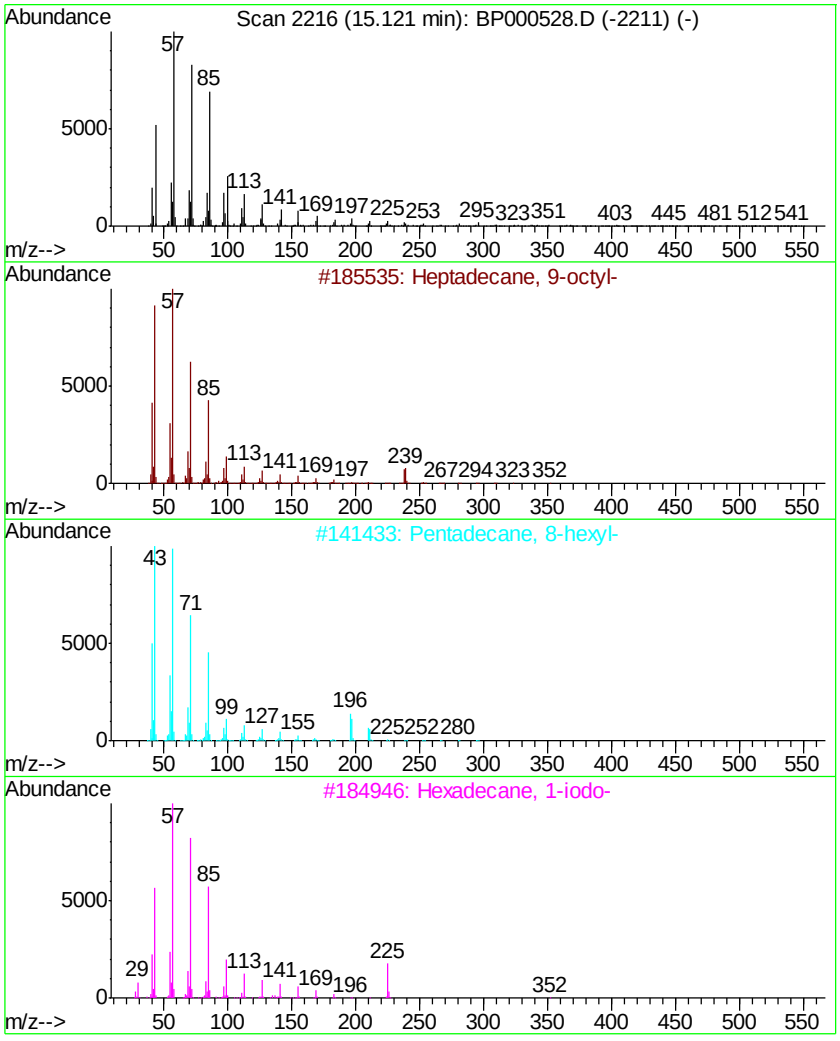
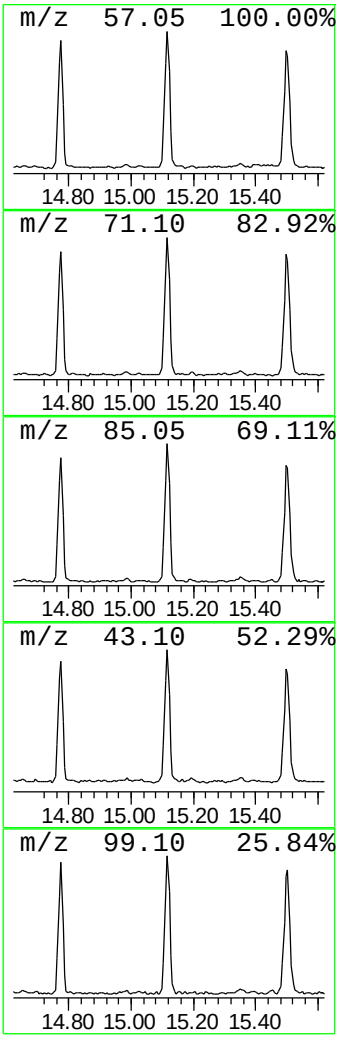
****

Peak Number 6 Heptadecane, 9-octyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.12	3.98 ng	251731	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	98
2	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	96
3	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	93
4	Heptadecane	240	C17H36	000629-78-7	93
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93





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ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : MW-104D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.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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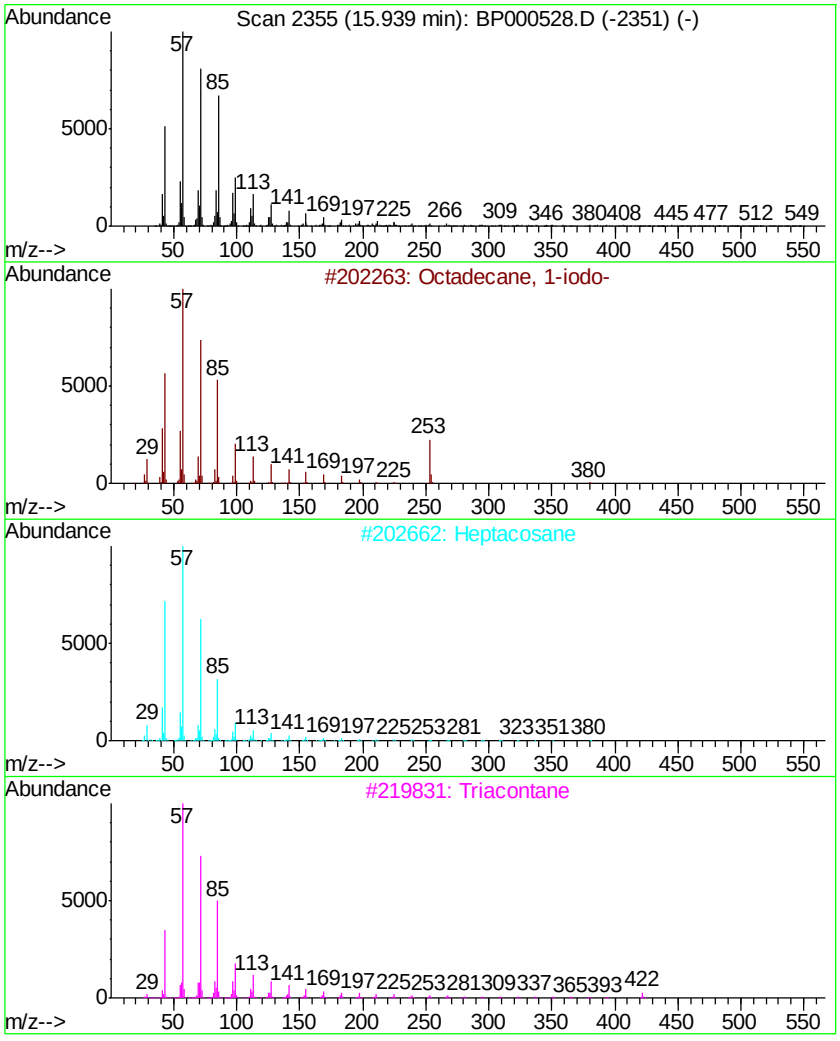
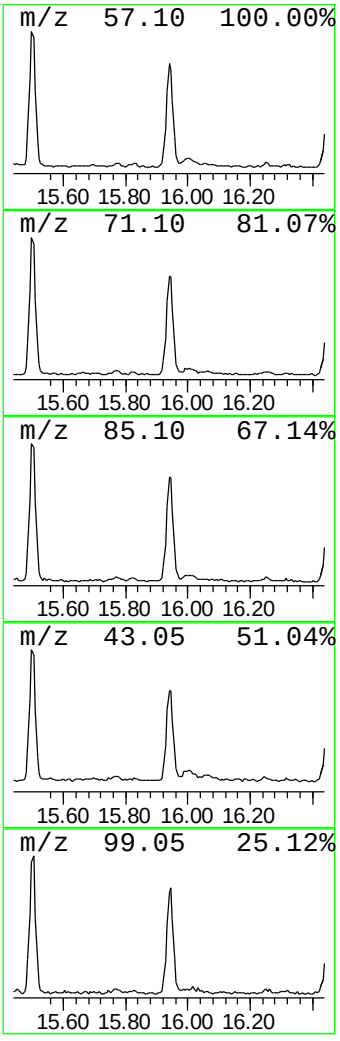
Peak Number 7 Octadecane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	3.55 ng	224790	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	98
2	Heptacosane	380	C27H56	000593-49-7	94
3	Triacontane	422	C30H62	000638-68-6	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	91





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Instrument : BNA_P
ClientSampleId : MW-104D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.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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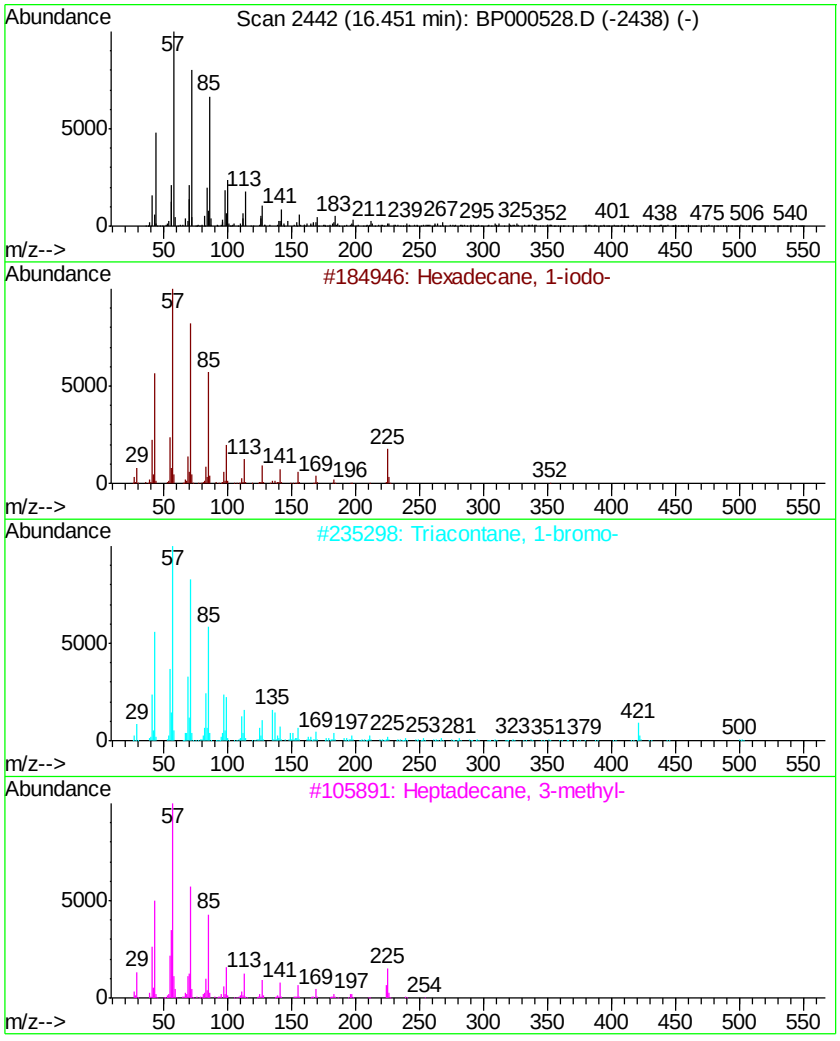
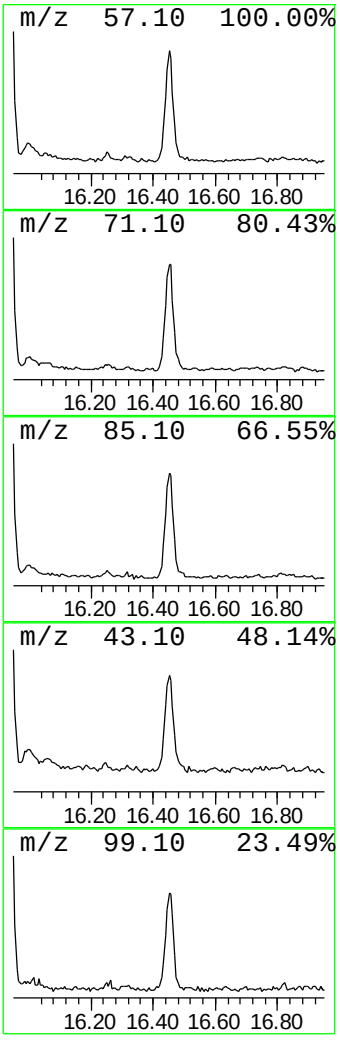
Peak Number 8 Hexadecane, 1-iodo- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.45	2.49 ng	157323	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	94
2	Triacontane, 1-bromo-	500	C30H61Br	004209-22-7	91
3	Heptadecane, 3-methyl-	254	C18H38	006418-44-6	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Hexatriacontane	507	C36H74	000630-06-8	86





Tentatively Identified Compound (LSC) summary

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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
unknown6.54	6.54	73.0	ng	5996390	1	6.77	1642050	20.0
n-Hexadecanoic acid	11.85	5.3	ng	654767	4	11.31	2478190	20.0
5-Eicosene, (E)-	13.83	8.0	ng	903353	5	13.97	2270100	20.0
Heneicosane	14.77	3.3	ng	210337	6	15.46	1265300	20.0
Heptadecane, 9-oc...	15.12	4.0	ng	251731	6	15.46	1265300	20.0
Octadecane, 1-iodo-	15.94	3.5	ng	224790	6	15.46	1265300	20.0
Hexadecane, 1-iodo-	16.45	2.5	ng	157323	6	15.46	1265300	20.0