LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104897.D
Acq On : 27 Apr 2018 22:26
Operator : JU/SJ
Sample : J2549-09
Misc :
ALS Vial : 19 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:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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	5.016	494	498	508	rVB	91269	126555	4.58%	0.519%
2	5.422	563	567	581	rBV	2413997	2699317	97.74%	11.072%
3	6.451	736	742	755	rBV	2361891	2737058	99.10%	11.227%
4	6.575	758	763	766	rBV	2941419	2761832	100.00%	11.328%
5	6.798	797	801	805	rBV	749124	590099	21.37%	2.420%
6	6.957	824	828	831	rBV	2468208	2130078	77.13%	8.737%
7	7.369	893	898	901	rBV	1743092	1654381	59.90%	6.786%
8	8.081	1016	1019	1036	rBV	747298	776782	28.13%	3.186%
9	9.157	1198	1202	1206	rBV	2730920	2692748	97.50%	11.045%
10	9.551	1265	1269	1277	rBV	241714	237033	8.58%	0.972%
11	9.763	1301	1305	1309	rBV	55365	47810	1.73%	0.196%
12	9.839	1314	1318	1322	rBV2	902812	774741	28.05%	3.178%
13	10.045	1350	1353	1357	rBV2	30763	33038	1.20%	0.136%
14	10.263	1387	1390	1392	rVB	69574	52954	1.92%	0.217%
15	10.633	1449	1453	1462	rBV	1622174	1646247	59.61%	6.752%
16	10.733	1467	1470	1475	rBV	62916	67162	2.43%	0.275%
17	11.186	1544	1547	1549	rBV	30811	29018	1.05%	0.119%
18	11.333	1568	1572	1574	rBV	717582	660185	23.90%	2.708%
19	11.351	1574	1575	1581	rVB	78546	74189	2.69%	0.304%
20	11.857	1656	1661	1669	rBV	411081	436860	15.82%	1.792%
21	12.551	1775	1779	1785	rBV	106537	118964	4.31%	0.488%
22	12.639	1791	1794	1802	rBV2	151728	158353	5.73%	0.650%
23	12.780	1812	1818	1821	rBV	88463	91417	3.31%	0.375%
24	12.851	1827	1830	1835	rVB	66895	56131	2.03%	0.230%
25	12.921	1837	1842	1845	rBV	2211984	2108545	76.35%	8.649%
26	13.192	1886	1888	1895	rVB	97608	89249	3.23%	0.366%
27	13.468	1933	1935	1940	rBV4	17439	29876	1.08%	0.123%
28	13.804	1989	1992	1995	rBV	88103	80461	2.91%	0.330%
29	13.839	1995	1998	2004	rVB	54254	60045	2.17%	0.246%
30	13.980	2018	2022	2025	rBV	678765	658287	23.84%	2.700%
31	14.080	2036	2039	2042	rVB	53147	47734	1.73%	0.196%
32	14.357	2084	2086	2093	rVB4	41232	46564	1.69%	0.191%
33	14.457	2101	2103	2106	rVB2	58831	50266	1.82%	0.206%
34	14.562	2118	2121	2126	rBV6	41161	53245	1.93%	0.218%

LSC Area Percent Report

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Integrator: RTE
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Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.445	2267	2271	2278	rBV	363023	502722	18.20%	2.062%

Sum of corrected areas: 24379946

LSC Report - Integrated Chromatogram

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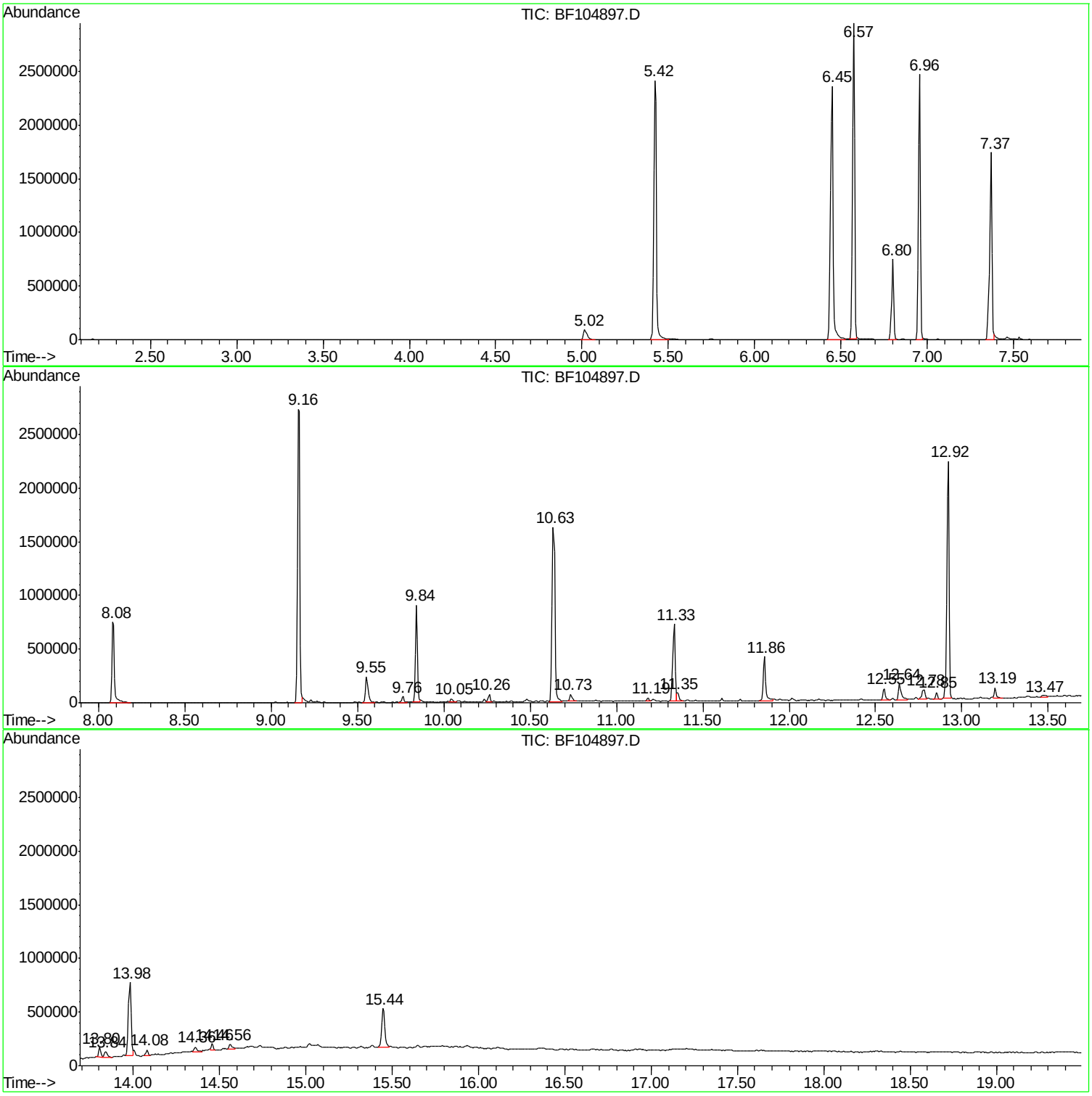
Sample : J2549-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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Data File : BF104897.D
Acq On : 27 Apr 2018 22:26
Operator : JU/SJ
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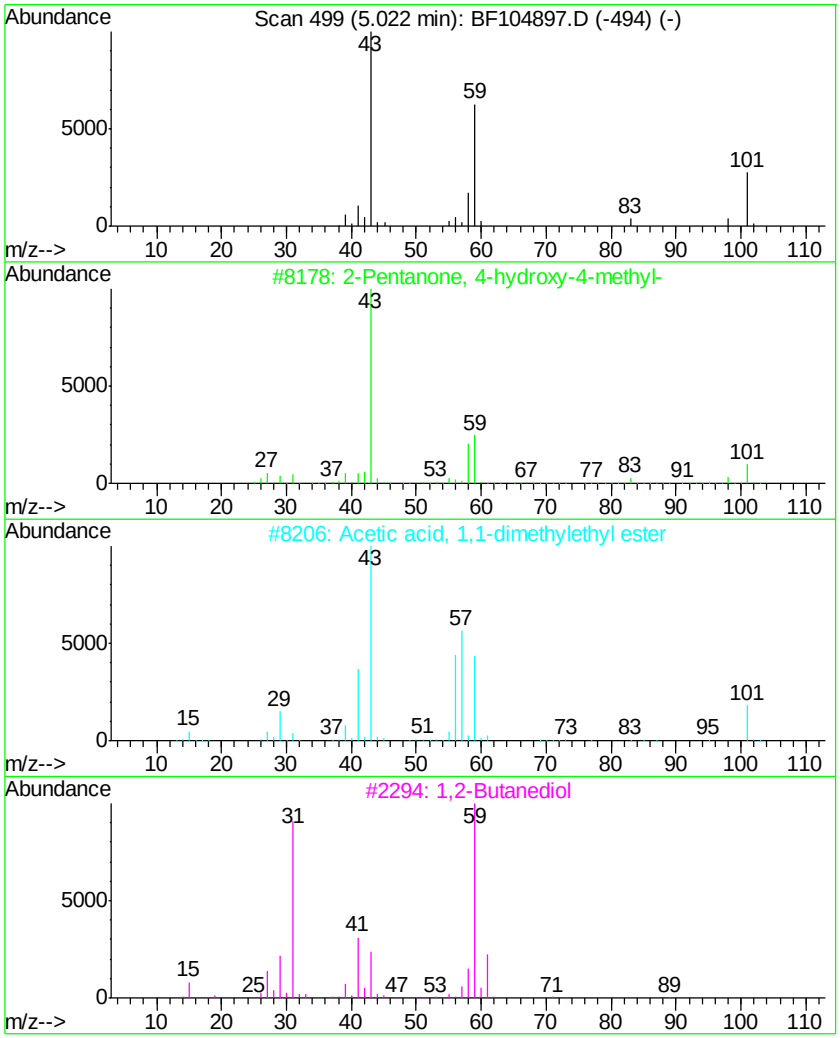
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

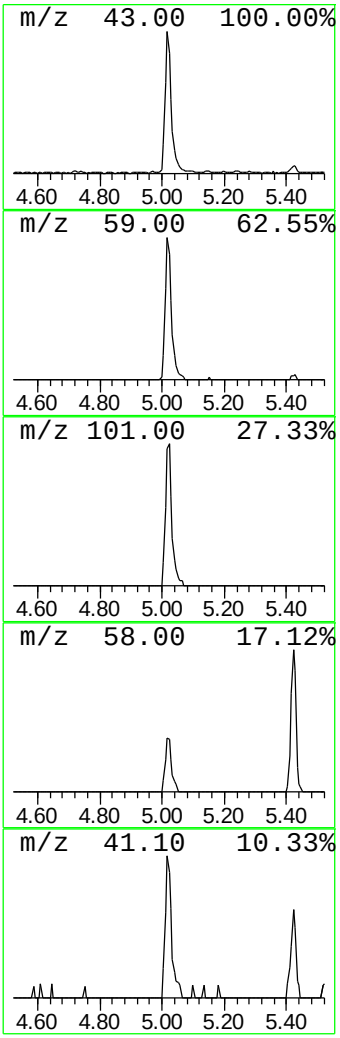
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	4.29 ng	126555	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50
3	1,2-Butanediol	90	C4H10O2	000584-03-2	32
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104897.D
Acq On : 27 Apr 2018 22:26
Operator : JU/SJ
Sample : J2549-09
Misc :
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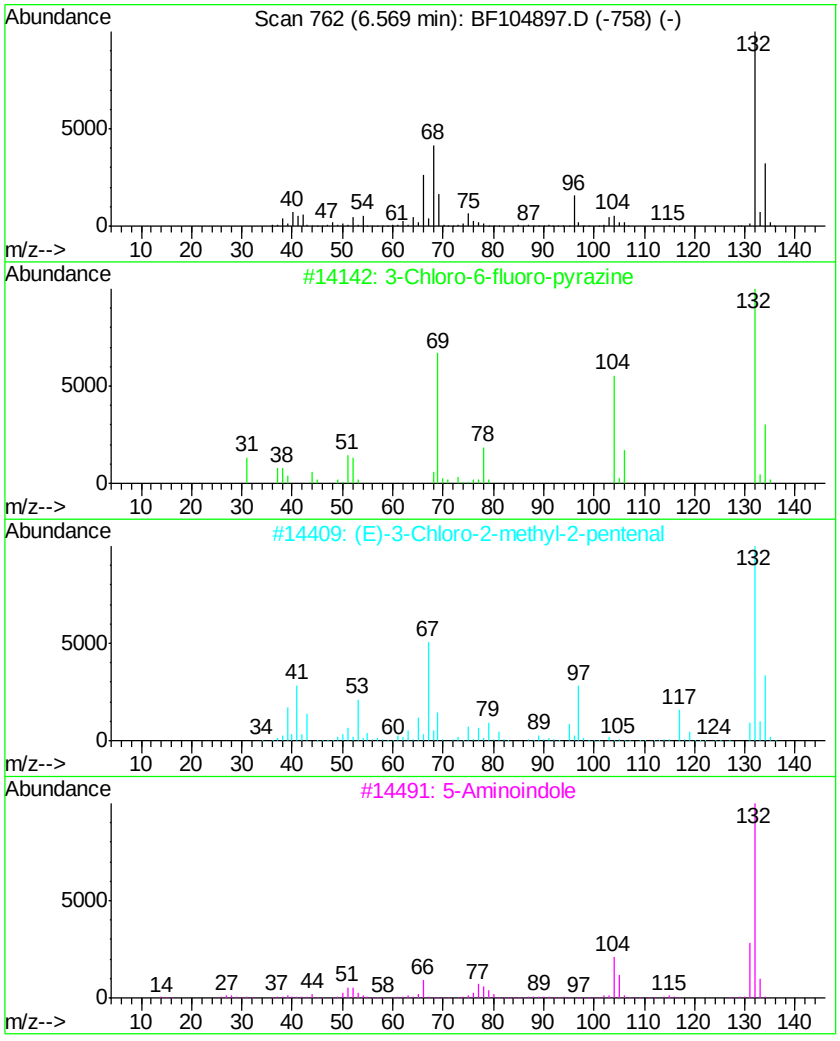
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

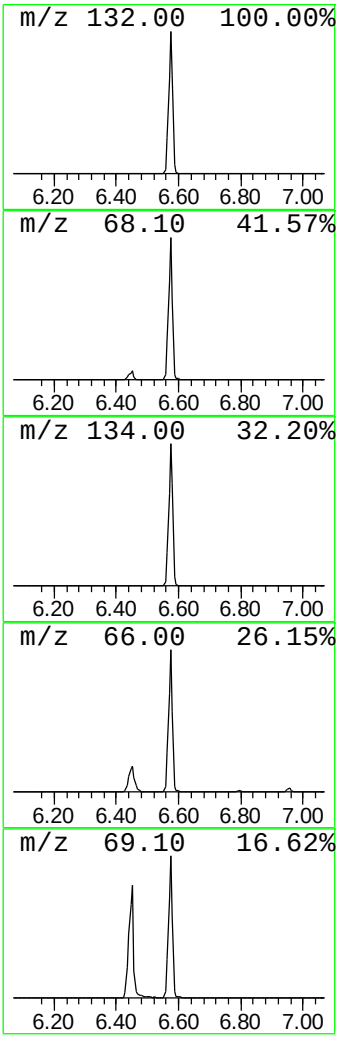
****

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	93.61 ng	2761830	1,4-Dichlorobenzene-d4	6.80

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	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





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Data File : BF104897.D
Acq On : 27 Apr 2018 22:26
Operator : JU/SJ
Sample : J2549-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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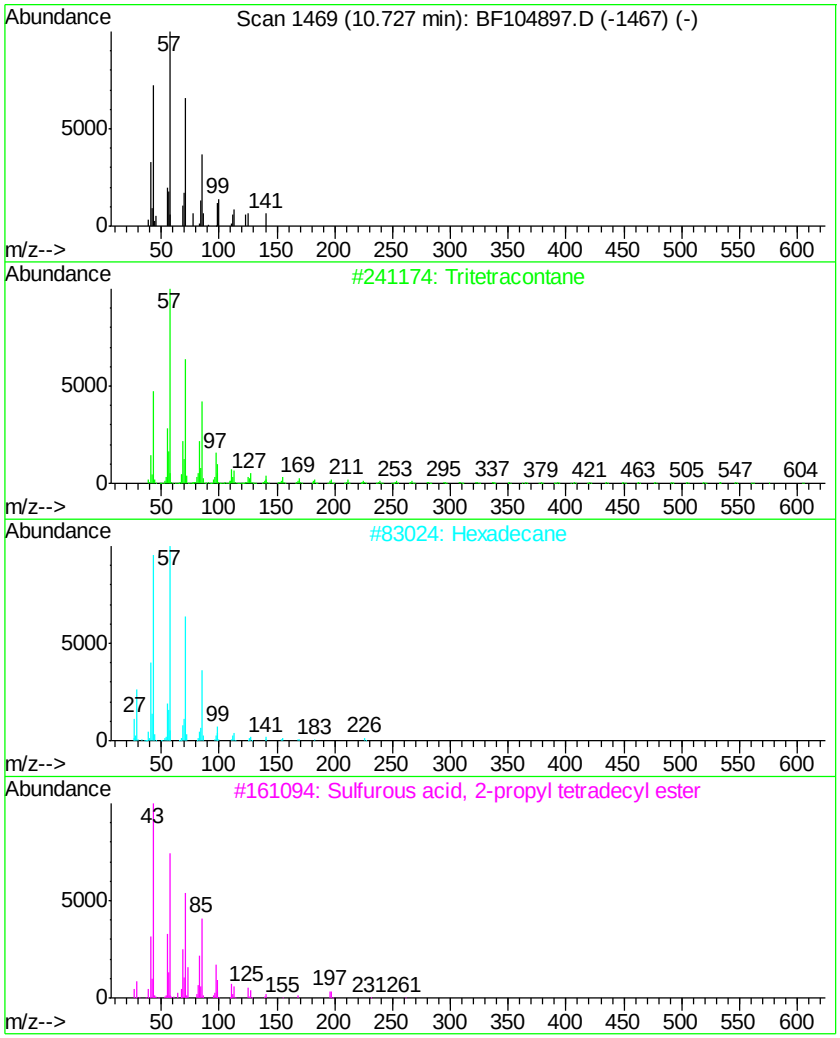
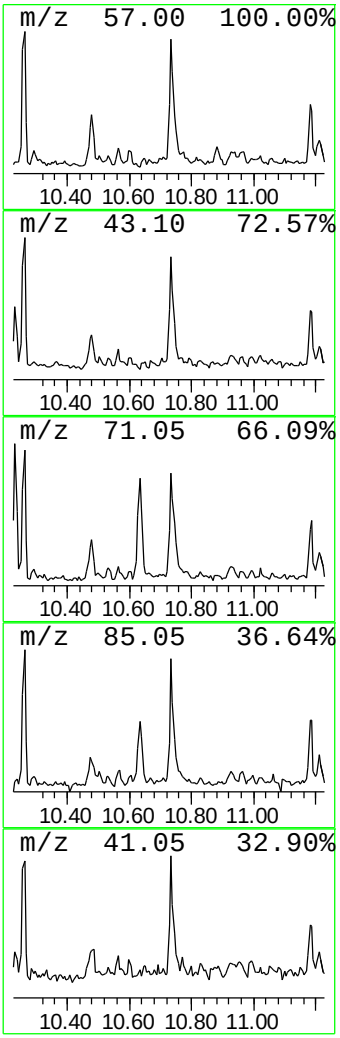
Peak Number 4 Tritetracontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.73	2.03 ng	67162	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tritetracontane	605	C43H88	007098-21-7	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	90
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	90
5	Nonadecane	268	C19H40	000629-92-5	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104897.D
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Operator : JU/SJ
Sample : J2549-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

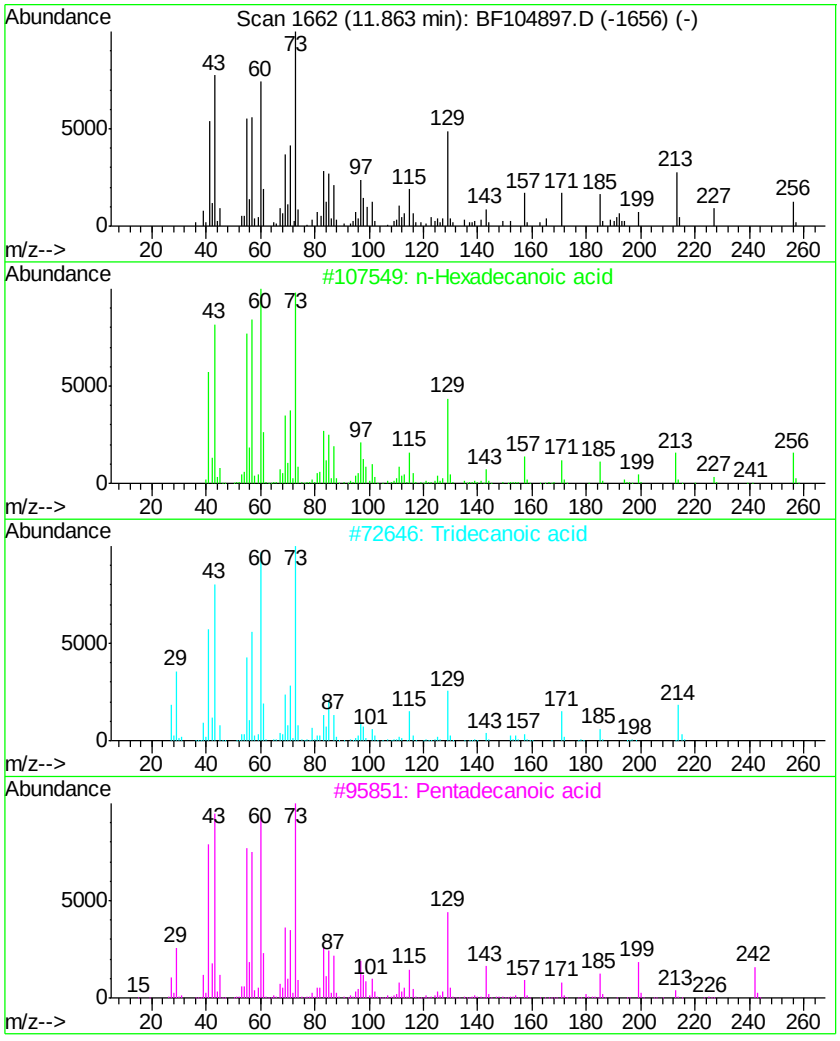
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

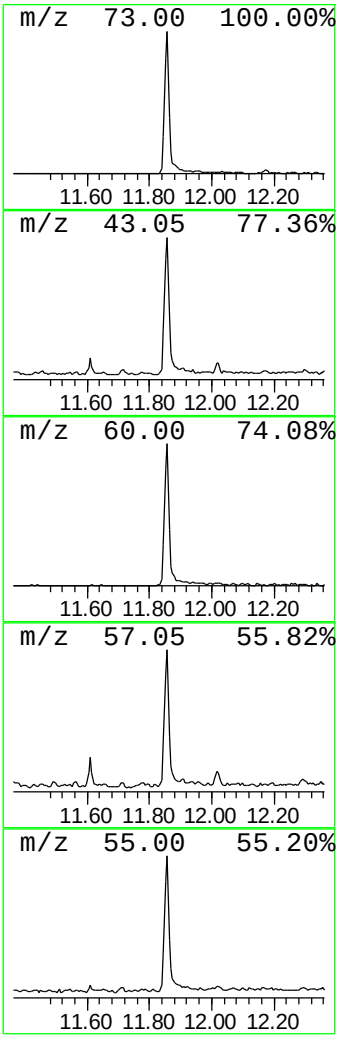
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	13.23 ng	436860	Phenanthrene-d10	11.33

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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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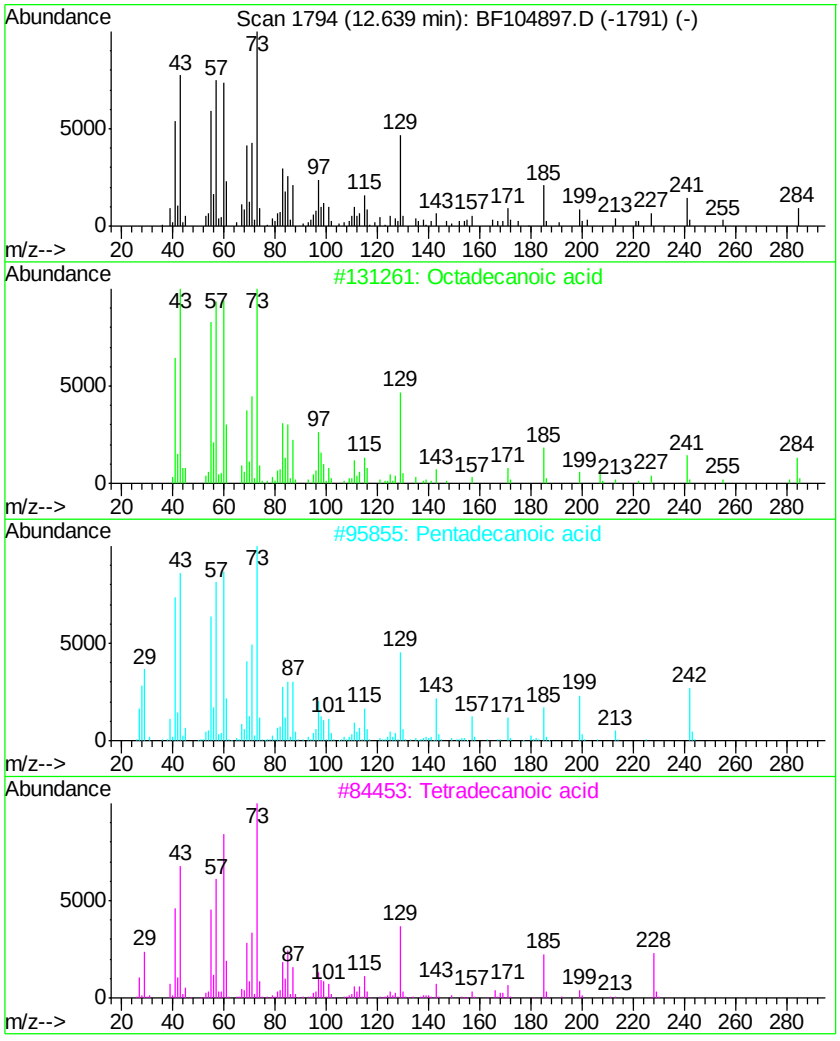
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

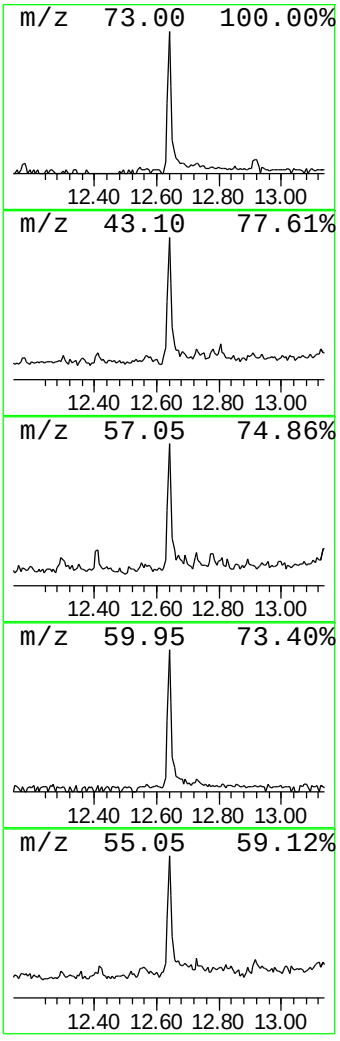
****

Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	4.80 ng	158353	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74





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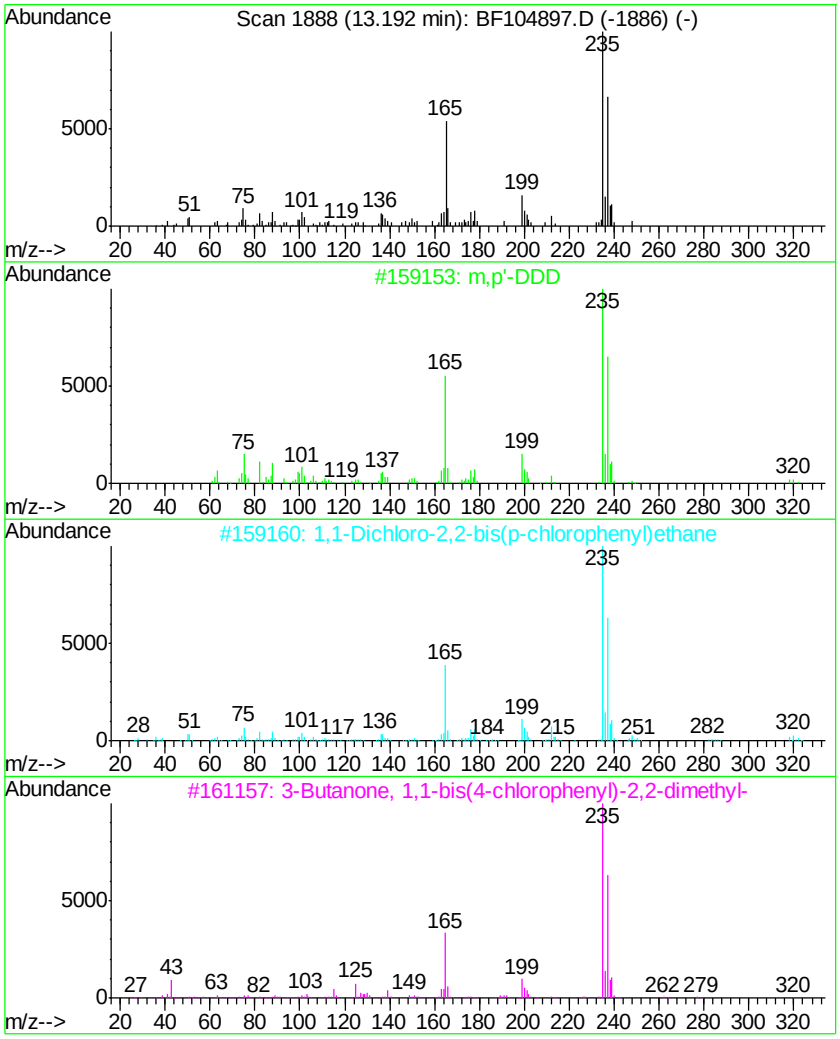
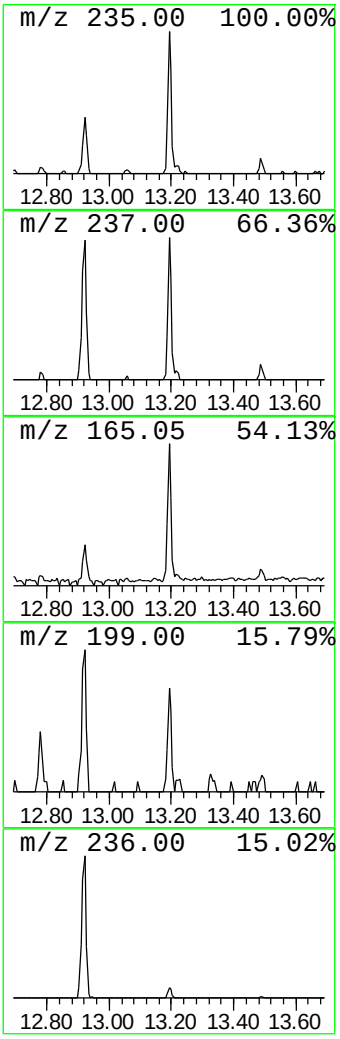
Peak Number 7 m,p'-DDD Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.19	2.71 ng	89249	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	m,p'-DDD	318	C14H10Cl4	004329-12-8	91
2	1,1-Dichloro-2,2-bis(p-chlorophe...	318	C14H10Cl4	000072-54-8	87
3	3-Butanone, 1,1-bis(4-chlorophen...	320	C18H18Cl2O	1000158-20-4	83
4	9H-Carbazole, 3,6-dichloro-	235	C12H7Cl2N	005599-71-3	53
5	1,2-Bis(2-chlorophenyl)-1,2-bis(...	470	C26H18Cl4	1000137-94-8	43





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

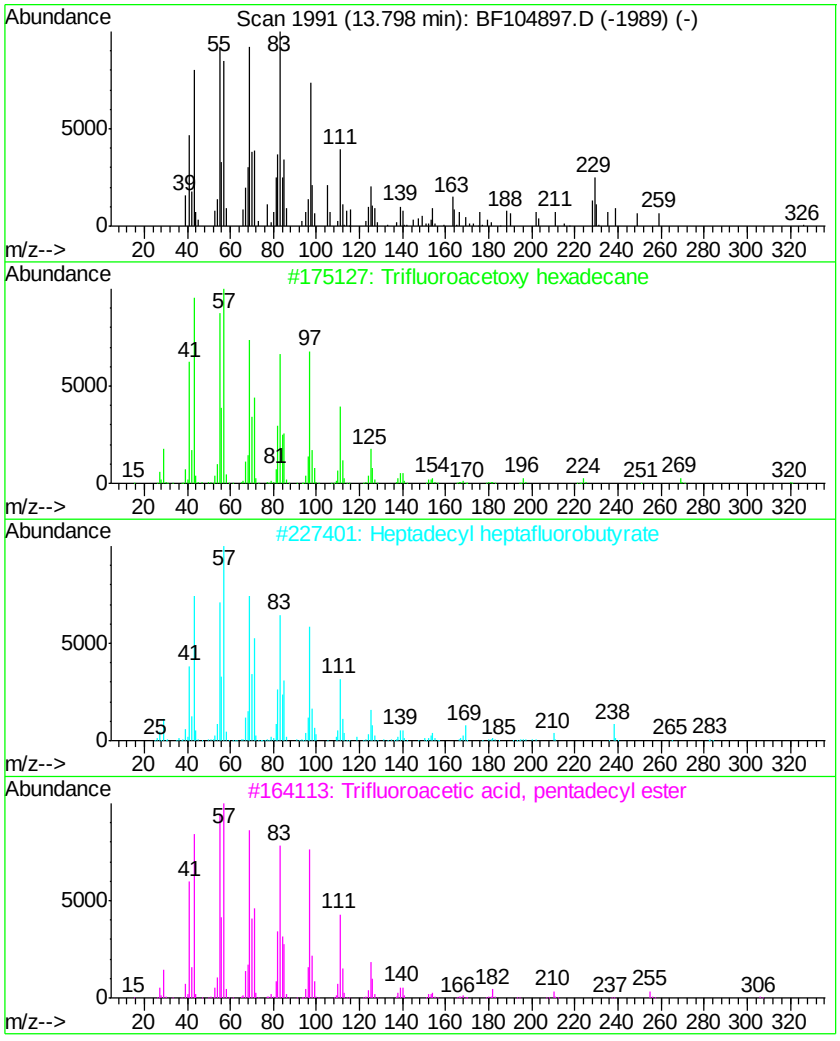
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

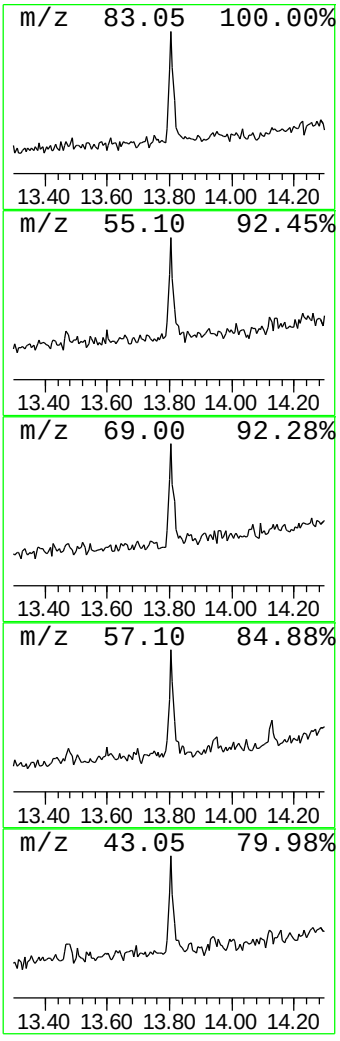
****

Peak Number 8 Trifluoroacetoxy hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	2.44 ng	80461	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	87
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	81





Tentatively Identified Compound (LSC) summary

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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...	5.02	4.3	ng	126555	1	6.80	590099	20.0
unknown6.57	6.57	93.6	ng	2761830	1	6.80	590099	20.0
Tritetracontane	10.73	2.0	ng	67162	4	11.33	660185	20.0
n-Hexadecanoic acid	11.86	13.2	ng	436860	4	11.33	660185	20.0
Octadecanoic acid	12.64	4.8	ng	158353	4	11.33	660185	20.0
m,p'-DDD	13.19	2.7	ng	89249	5	13.98	658287	20.0
Trifluoroacetoxy ...	13.80	2.4	ng	80461	5	13.98	658287	20.0