LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021519\
Data File : BF112588.D
Acq On : 15 Feb 2019 19:37
Operator : JU/SJ
Sample : K1346-09 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-021419-B

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	5.040	498	502	511	rBV	28087	38146	3.11%	0.280%
2	5.463	571	574	592	rBV	704604	909585	74.05%	6.671%
3	6.481	744	747	765	rBV	809935	1007064	81.99%	7.386%
4	6.610	765	769	775	rBV	1085717	1070487	87.15%	7.851%
5	6.828	803	806	815	rBV	605874	538927	43.87%	3.953%
6	6.987	829	833	847	rBV	932354	814658	66.32%	5.975%
7	7.393	899	902	914	rBV	600504	645700	52.57%	4.736%
8	8.116	1021	1025	1033	rVB	668502	665153	54.15%	4.878%
9	8.698	1121	1124	1128	rBV	30090	23669	1.93%	0.174%
10	9.187	1203	1207	1217	rBV	1366690	1228344	100.00%	9.009%
11	9.263	1217	1220	1223	rVB	28186	24074	1.96%	0.177%
12	9.528	1260	1265	1269	rBV4	11781	18171	1.48%	0.133%
13	9.581	1271	1274	1281	rVB	60857	61472	5.00%	0.451%
14	9.792	1304	1310	1314	rVB	23115	22148	1.80%	0.162%
15	9.869	1319	1323	1332	rVB	967506	895652	72.92%	6.569%
16	10.292	1387	1395	1399	rBV4	20212	25640	2.09%	0.188%
17	10.422	1414	1417	1421	rVB	14869	15422	1.26%	0.113%
18	10.663	1455	1458	1468	rBV	831206	858304	69.87%	6.295%
19	11.210	1544	1551	1554	rBV3	14277	16089	1.31%	0.118%
20	11.357	1573	1576	1579	rBV	868744	863846	70.33%	6.336%
21	11.380	1579	1580	1585	rVV	105091	104927	8.54%	0.770%
22	11.439	1587	1590	1595	rVB2	13938	16521	1.34%	0.121%
23	11.875	1657	1664	1672	rBV4	111144	192547	15.68%	1.412%
24	11.975	1678	1681	1684	rBV2	33100	38636	3.15%	0.283%
25	12.157	1709	1712	1714	rBV2	11993	13302	1.08%	0.098%
26	12.298	1732	1736	1740	rBV7	10658	21115	1.72%	0.155%
27	12.416	1751	1756	1758	rBV	42217	51717	4.21%	0.379%
28	12.439	1758	1760	1764	rVV5	21935	29879	2.43%	0.219%
29	12.504	1768	1771	1773	rBV3	13706	20300	1.65%	0.149%
30	12.580	1780	1784	1787	rBV	112763	107845	8.78%	0.791%
31	12.663	1795	1798	1804	rBV6	35312	55917	4.55%	0.410%
32	12.733	1806	1810	1812	rBV5	13979	21073	1.72%	0.155%
33	12.810	1817	1823	1828	rBV	128261	156484	12.74%	1.148%
34	12.863	1830	1832	1835	rBV4	17429	17761	1.45%	0.130%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
ClientSampleId : CL-01-021419-B

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

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Peak separation: 5

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

35	12.939	1841	1845	1848	rBV	1274303	1062454	86.49%	7.792%
36	13.157	1881	1882	1885	rVB2	18819	14584	1.19%	0.107%
37	13.339	1910	1913	1915	rBV2	18360	17649	1.44%	0.129%
38	13.498	1938	1940	1945	rVB6	26278	27139	2.21%	0.199%
39	13.827	1993	1996	2000	rBV2	88940	93495	7.61%	0.686%
40	14.010	2023	2027	2030	rBV	789344	754674	61.44%	5.535%
41	14.145	2048	2050	2052	rBV	46788	32869	2.68%	0.241%
42	14.451	2099	2102	2105	rBV	83190	89906	7.32%	0.659%
43	14.751	2151	2153	2157	rVB	68674	65158	5.30%	0.478%
44	15.086	2208	2210	2215	rVB	150649	135460	11.03%	0.993%
45	15.492	2275	2279	2283	rVB2	498256	606264	49.36%	4.446%
46	15.892	2344	2347	2353	rVB2	103055	144616	11.77%	1.061%

Sum of corrected areas: 13634843

LSC Report - Integrated Chromatogram

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Misc :
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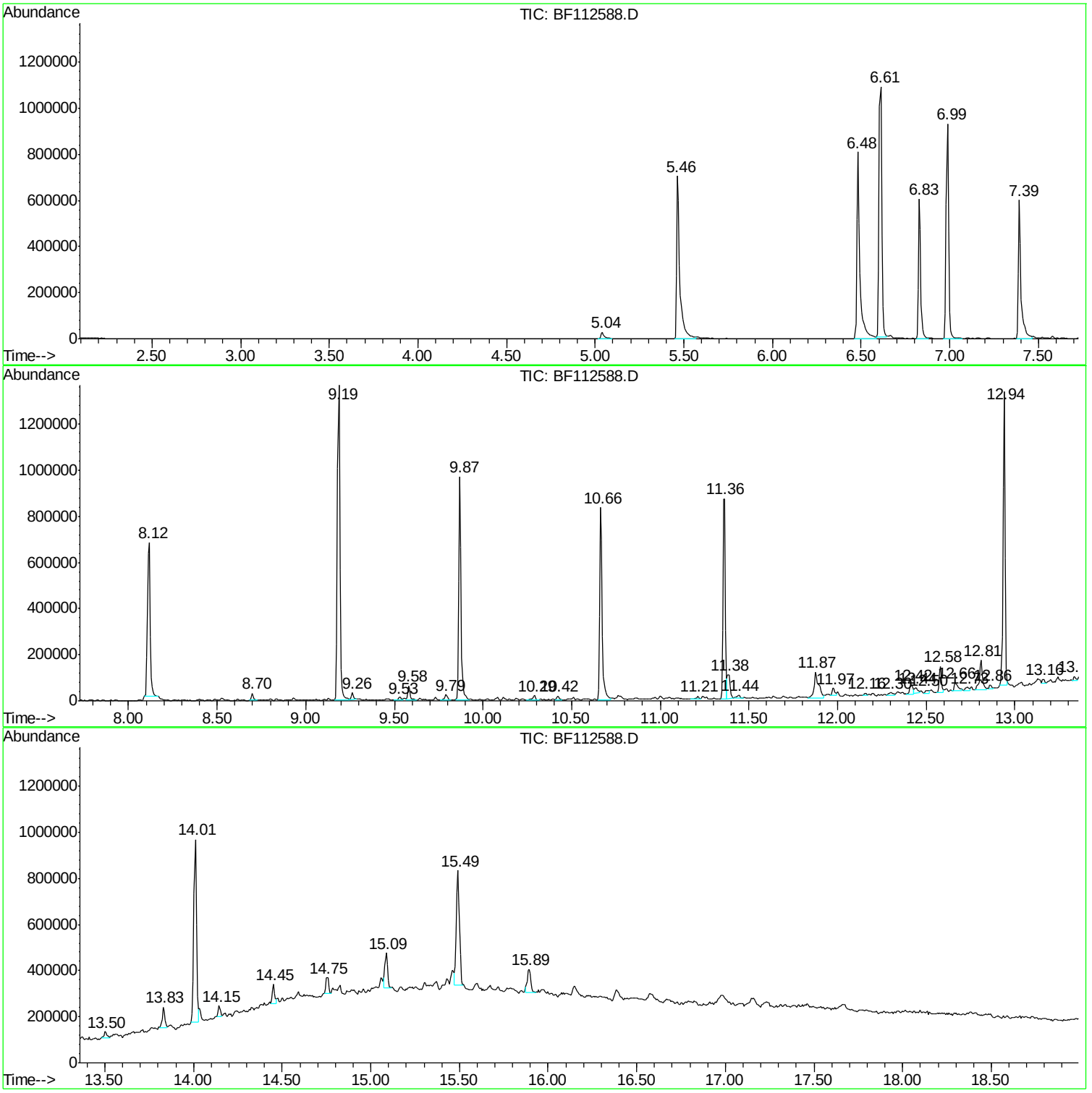
Instrument : BNA_F
ClientSampleId : CL-01-021419-B

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021519\
Data File : BF112588.D
Acq On : 15 Feb 2019 19:37
Operator : JU/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : CL-01-021419-B

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

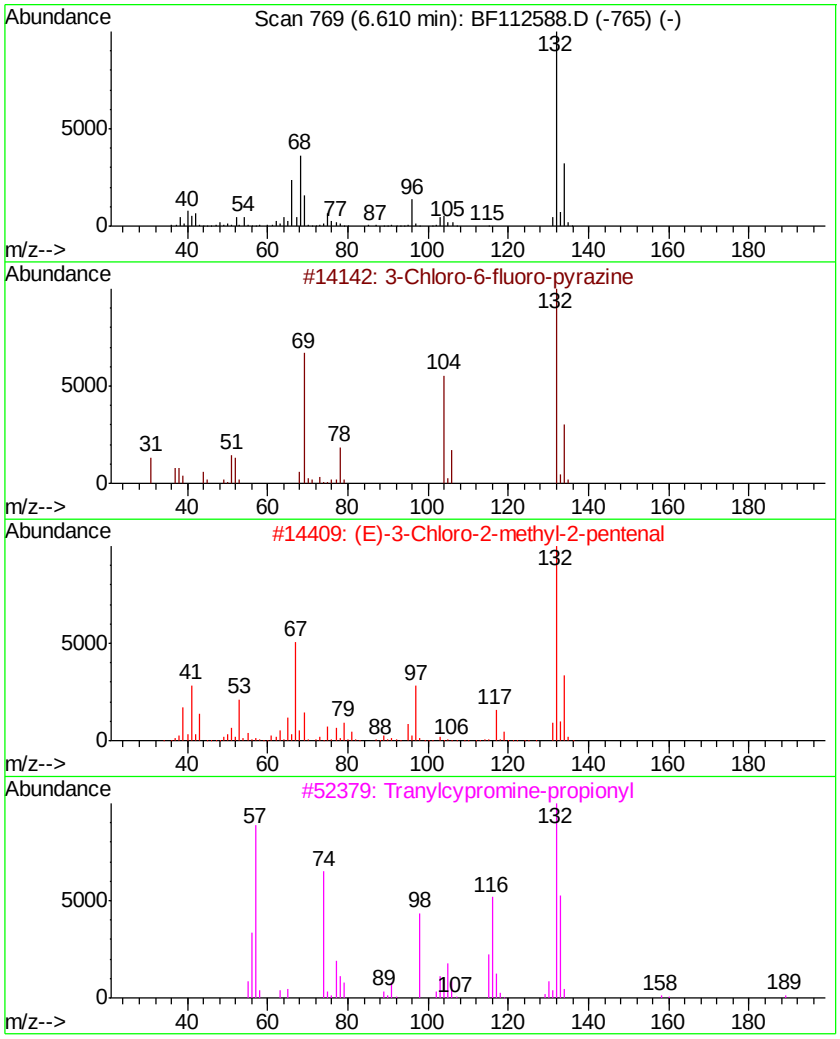
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

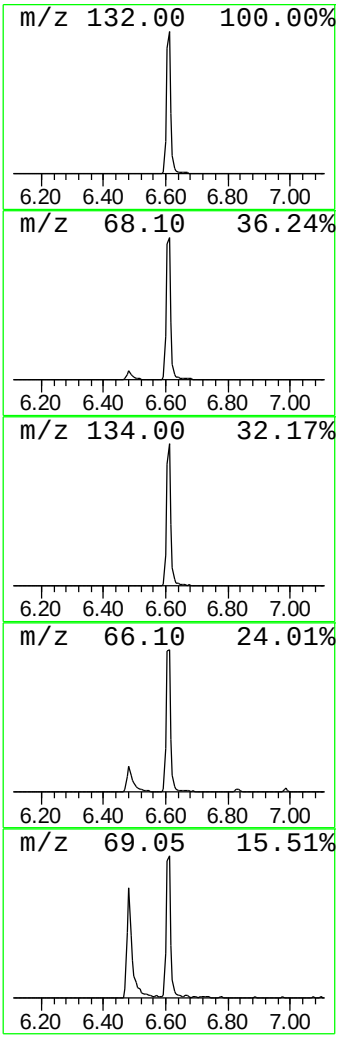
****

Peak Number 1 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	39.73 ng	1070490	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : CL-01-021419-B

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

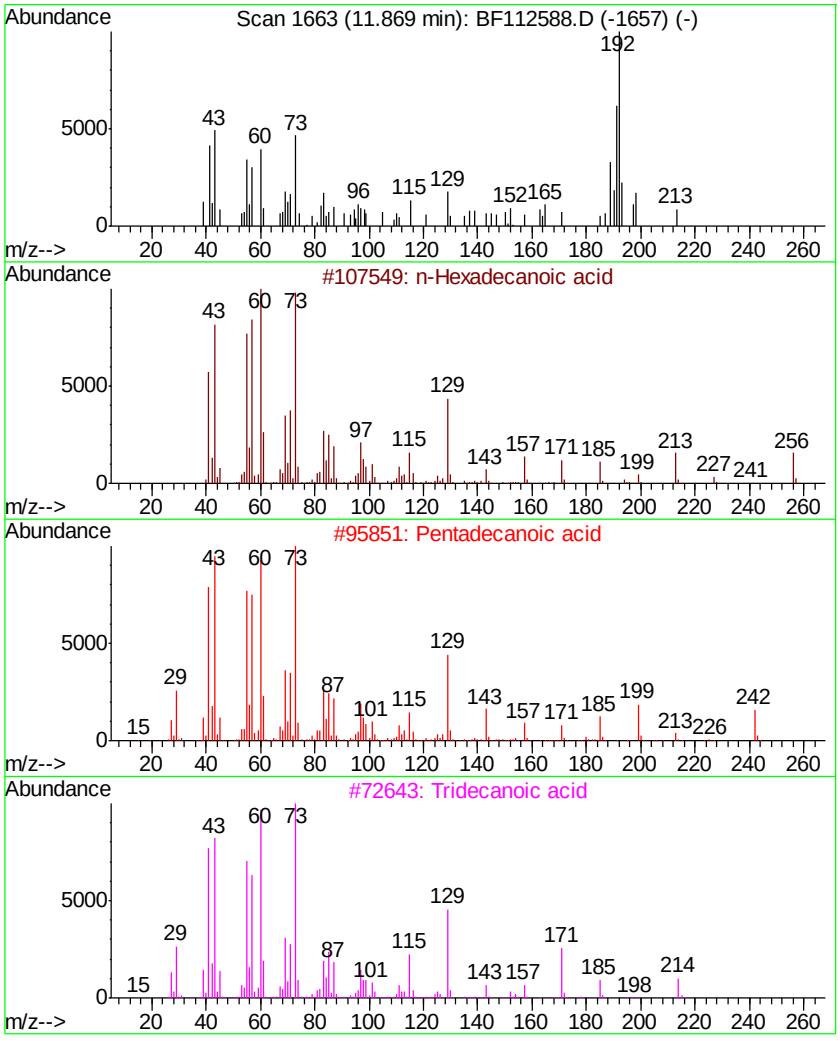
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

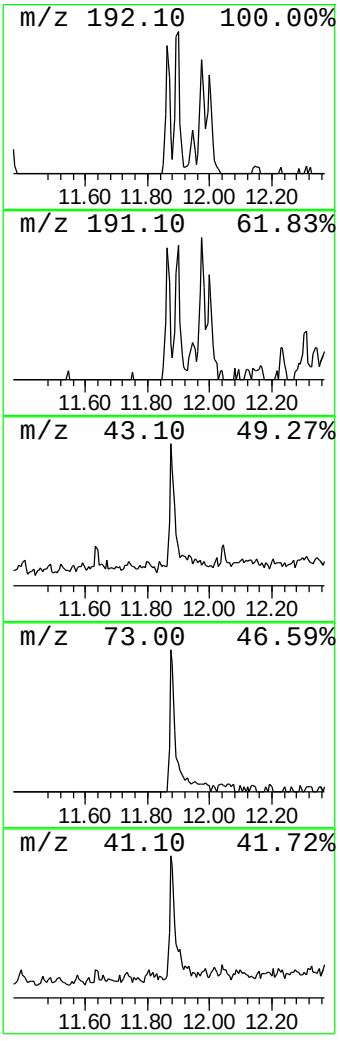
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	4.46 ng	192547	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	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	68
4	Dodecanoic acid	200	C12H24O2	000143-07-7	58
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	53





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Instrument : BNA_F
ClientSampleId : CL-01-021419-B

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

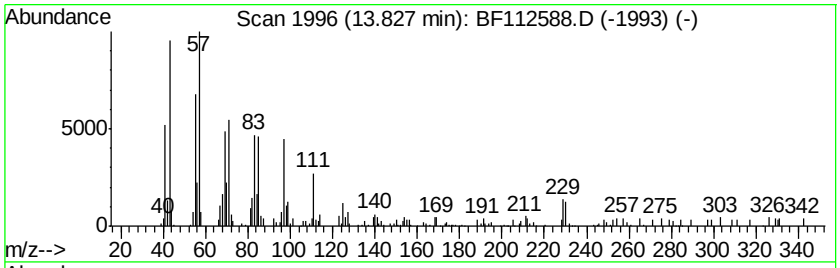
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

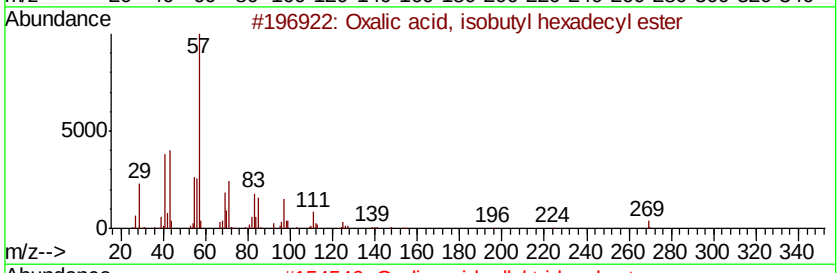
****

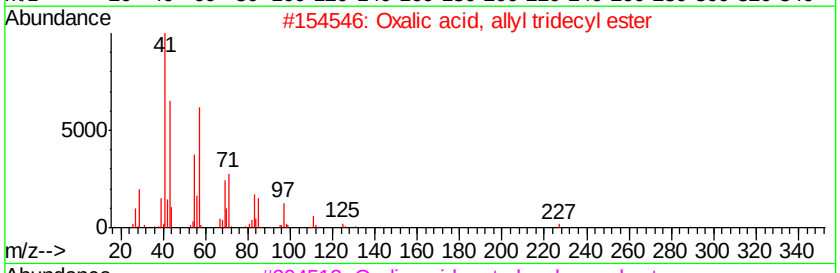
Peak Number 4 Oxalic acid, isobutyl hexad... Concentration Rank 6

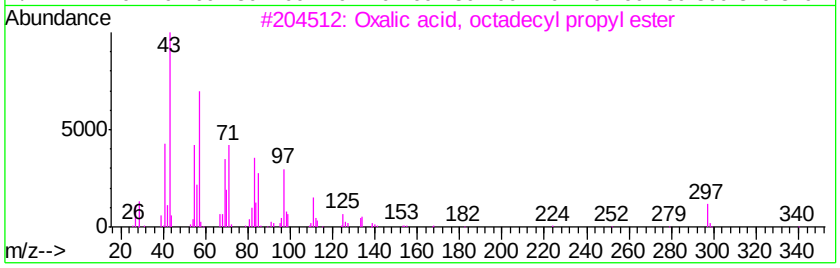
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	2.48 ng	93495	Chrysene-d12	14.01

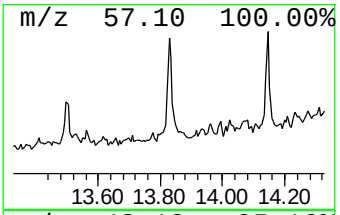
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	83
2	Oxalic acid, allyl tridecyl ester	312	C18H32O4	1000309-24-1	83
3	Oxalic acid, octadecyl propyl ester	384	C23H44O4	1000309-27-0	83
4	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	81
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	74

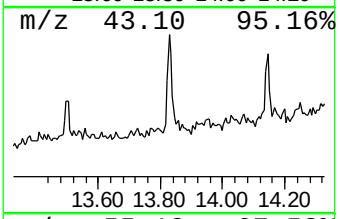


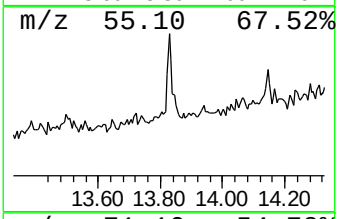


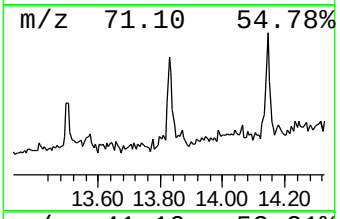


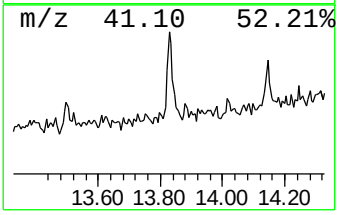












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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

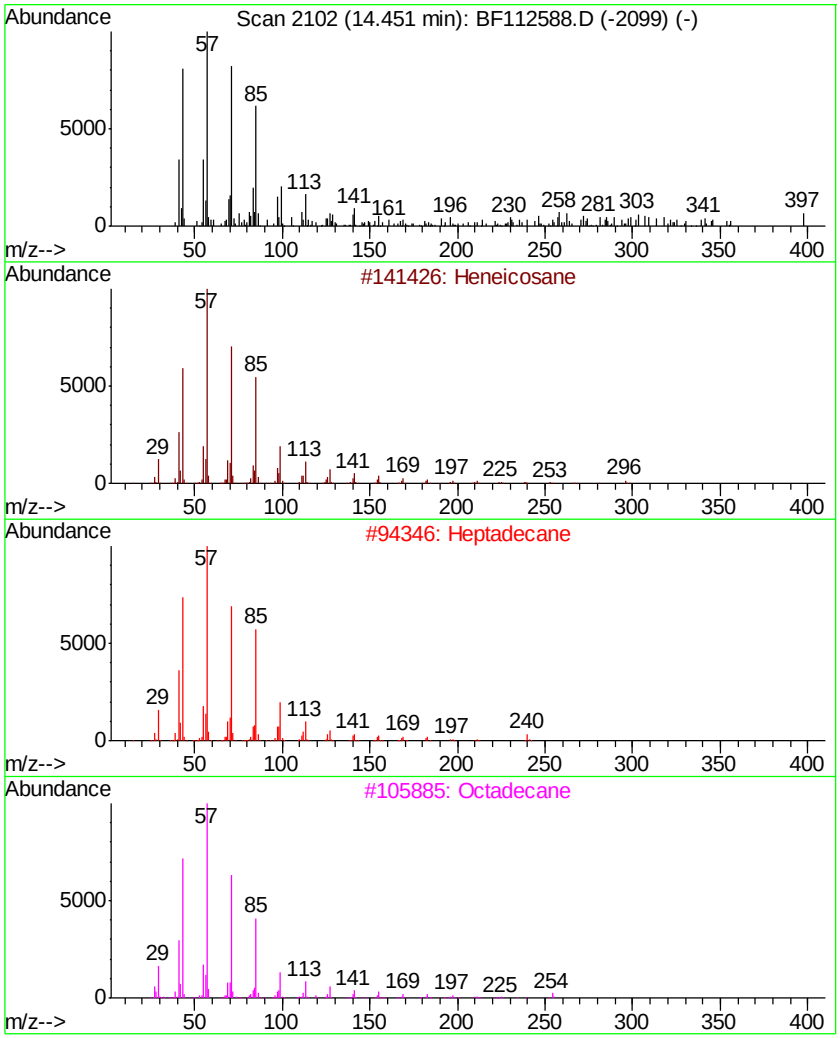
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

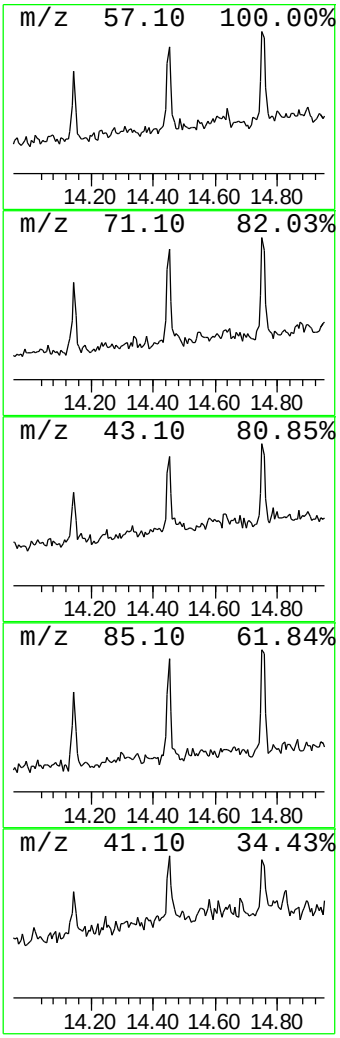
****

Peak Number 5 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	2.38 ng	89906	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	97
2	Heptadecane	240	C17H36	000629-78-7	90
3	Octadecane	254	C18H38	000593-45-3	76
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	76
5	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	74





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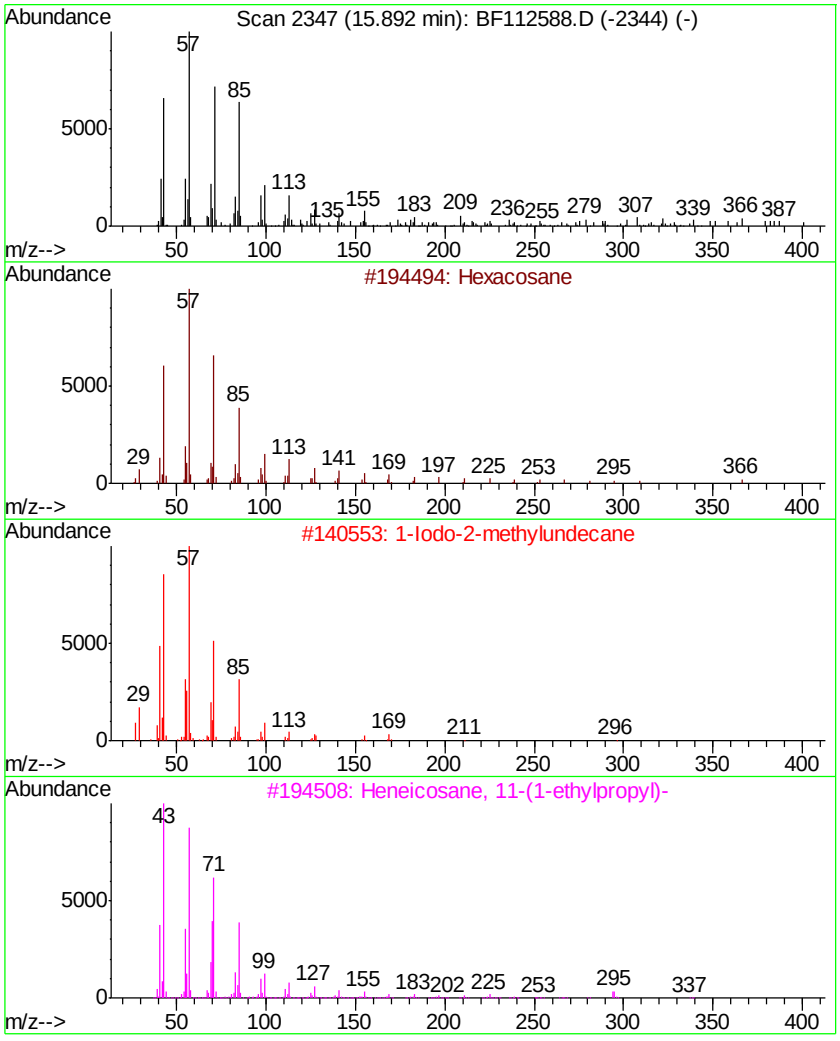
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

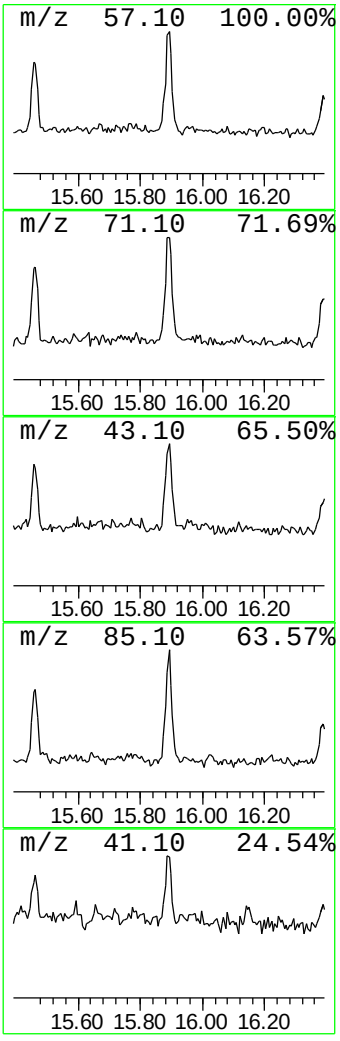
****

Peak Number 7 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.89	4.77 ng	144616	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	81
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	74
4	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	72
5	2-methyloctacosane	408	C29H60	1000376-72-8	72





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
unknown6.61	6.61	39.7	ng	1070490	1	6.83	538927	20.0
n-Hexadecanoic acid	11.87	4.5	ng	192547	4	11.36	863846	20.0
Oxalic acid, isob...	13.83	2.5	ng	93495	5	14.01	754674	20.0
Heneicosane	14.45	2.4	ng	89906	5	14.01	754674	20.0
Hexacosane	15.89	4.8	ng	144616	6	15.49	606264	20.0