LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021519\
Data File : BF112589.D
Acq On : 15 Feb 2019 20:04
Operator : JU/SJ
Sample : K1346-11 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

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

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	510	rBV	37734	50573	3.10%	0.291%
2	5.463	571	574	595	rBV	919992	1096436	67.28%	6.316%
3	6.075	675	678	684	rBV3	15132	19761	1.21%	0.114%
4	6.357	723	726	729	rBV2	24188	23042	1.41%	0.133%
5	6.481	744	747	760	rBV	1058230	1218091	74.74%	7.017%
6	6.610	765	769	775	rVV	1352284	1301361	79.85%	7.497%
7	6.663	775	778	781	rVV2	59276	51299	3.15%	0.296%
8	6.828	803	806	813	rVB	711506	652136	40.02%	3.757%
9	6.987	828	833	842	rBV	1147935	1018285	62.48%	5.866%
10	7.104	847	853	855	rVB4	23984	28732	1.76%	0.166%
11	7.216	869	872	876	rVB3	22879	27576	1.69%	0.159%
12	7.363	891	897	899	rBV6	17272	26337	1.62%	0.152%
13	7.392	899	902	906	rVV	754872	751816	46.13%	4.331%
14	7.422	906	907	911	rVV	128638	96306	5.91%	0.555%
15	7.475	914	916	919	rVB3	22199	20316	1.25%	0.117%
16	7.534	919	926	929	rBV4	9201	19240	1.18%	0.111%
17	7.857	978	981	986	rBV5	17252	21035	1.29%	0.121%
18	8.092	1017	1021	1022	rBV	52683	47652	2.92%	0.275%
19	8.116	1022	1025	1032	rVV	919730	904830	55.52%	5.212%
20	8.169	1032	1034	1037	rVB2	29358	27596	1.69%	0.159%
21	8.698	1121	1124	1128	rBV	45421	37075	2.27%	0.214%
22	9.186	1203	1207	1216	rBV	1959377	1629674	100.00%	9.388%
23	9.263	1216	1220	1223	rVV	45342	39443	2.42%	0.227%
24	9.580	1271	1274	1282	rVB	74328	87756	5.38%	0.506%
25	9.792	1304	1310	1314	rBV	36774	32090	1.97%	0.185%
26	9.869	1319	1323	1337	rVB	1261913	1160104	71.19%	6.683%
27	10.292	1387	1395	1398	rBV4	37577	41548	2.55%	0.239%
28	10.422	1414	1417	1424	rVB2	17233	21768	1.34%	0.125%
29	10.663	1455	1458	1468	rBV	1073090	1136150	69.72%	6.545%
30	10.763	1472	1475	1480	rVB2	33113	43209	2.65%	0.249%
31	11.210	1548	1551	1554	rBV2	33917	27785	1.70%	0.160%
32	11.363	1573	1577	1579	rBV	1243321	1114411	68.38%	6.420%
33	11.386	1579	1581	1585	rVV	132737	127045	7.80%	0.732%
34	11.439	1587	1590	1595	rVB	16886	21579	1.32%	0.124%

LSC Area Percent Report

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Operator : JU/SJ
Sample : K1346-11 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

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

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

35	11.639	1621	1624	1627	rVB	27691	24415	1.50%	0.141%
36	11.874	1659	1664	1672	rBV4	116300	185696	11.39%	1.070%
37	11.974	1678	1681	1684	rBV2	31174	32028	1.97%	0.184%
38	12.045	1690	1693	1697	rVB	28610	26552	1.63%	0.153%
39	12.416	1753	1756	1758	rBV3	31742	40941	2.51%	0.236%
40	12.580	1780	1784	1788	rBV	151206	150981	9.26%	0.870%
41	12.663	1796	1798	1803	rBV3	25280	35190	2.16%	0.203%
42	12.810	1817	1823	1829	rBV2	142416	191114	11.73%	1.101%
43	12.939	1839	1845	1849	rBV	1727956	1481406	90.90%	8.534%
44	13.121	1873	1876	1877	rBV3	18058	19204	1.18%	0.111%
45	13.157	1880	1882	1885	rVB	41206	36758	2.26%	0.212%
46	13.504	1937	1941	1945	rBV	60051	80610	4.95%	0.464%
47	13.833	1993	1997	2008	rBV3	139267	182835	11.22%	1.053%
48	14.010	2023	2027	2030	rBV	903227	881453	54.09%	5.078%
49	14.145	2047	2050	2053	rBV	99549	92852	5.70%	0.535%
50	14.451	2099	2102	2106	rBV	117648	109850	6.74%	0.633%
51	14.751	2151	2153	2157	rVB	104471	101353	6.22%	0.584%
52	15.086	2208	2210	2214	rVB	133144	128525	7.89%	0.740%
53	15.492	2275	2279	2283	rVB	510582	635674	39.01%	3.662%

Sum of corrected areas: 17359494

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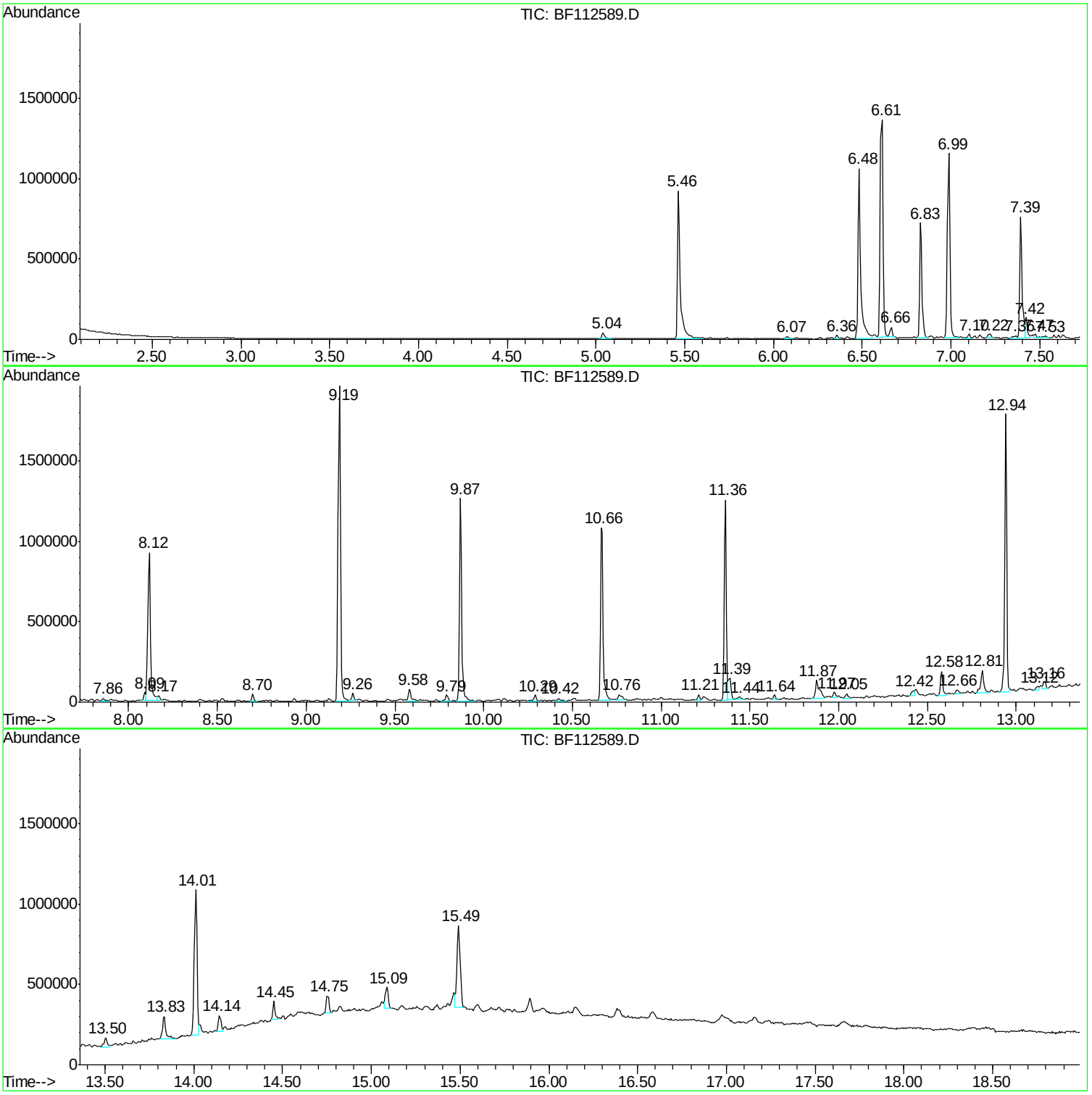
Misc :
ALS Vial : 13 Sample Multiplier: 1

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

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

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

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

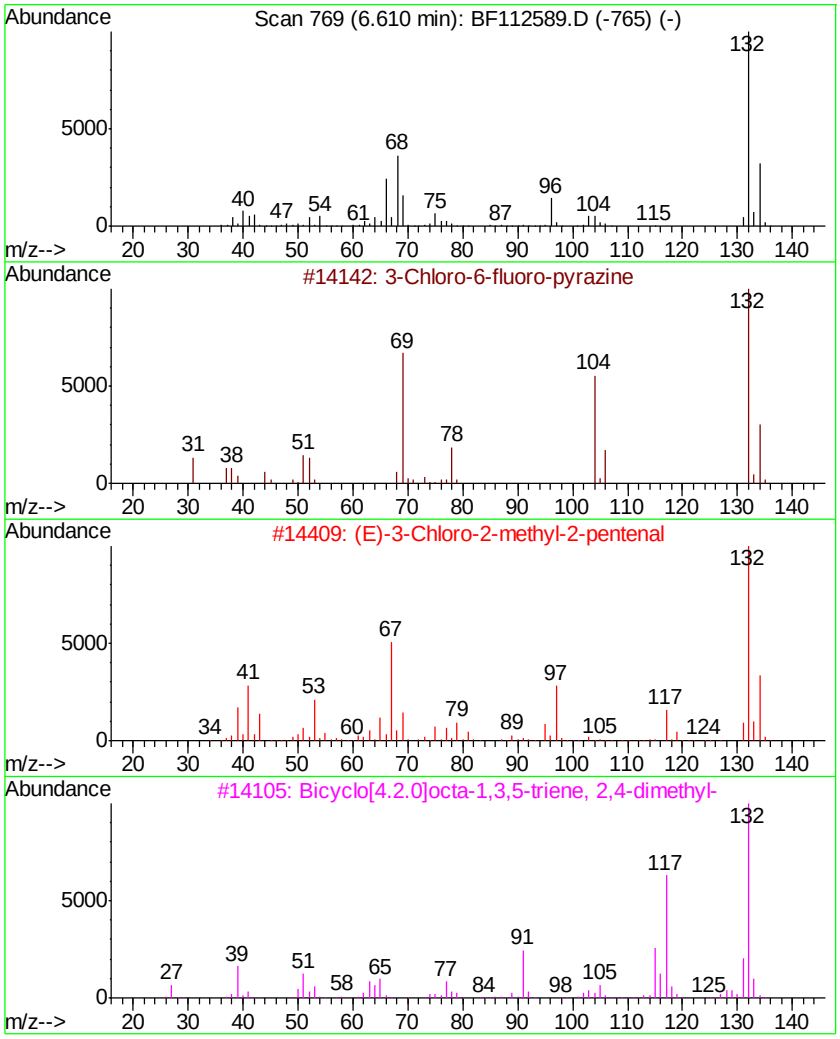
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

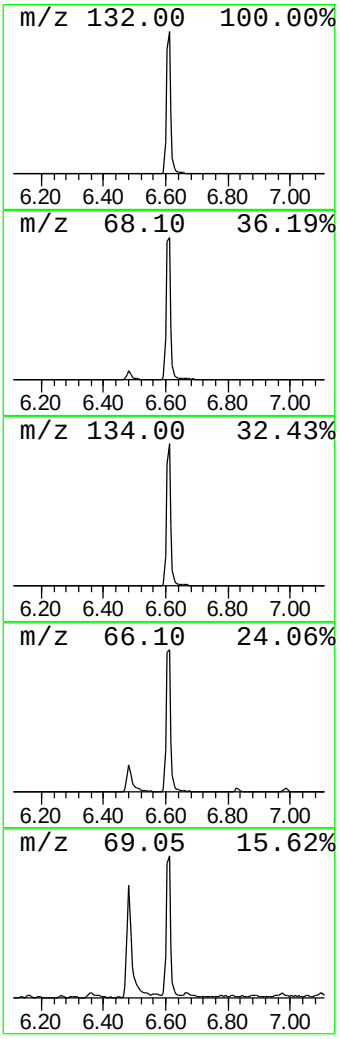
****

Peak Number 1 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	39.91 ng	1301360	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	17
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

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Data File : BF112589.D
Acq On : 15 Feb 2019 20:04
Operator : JU/SJ
Sample : K1346-11 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

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

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

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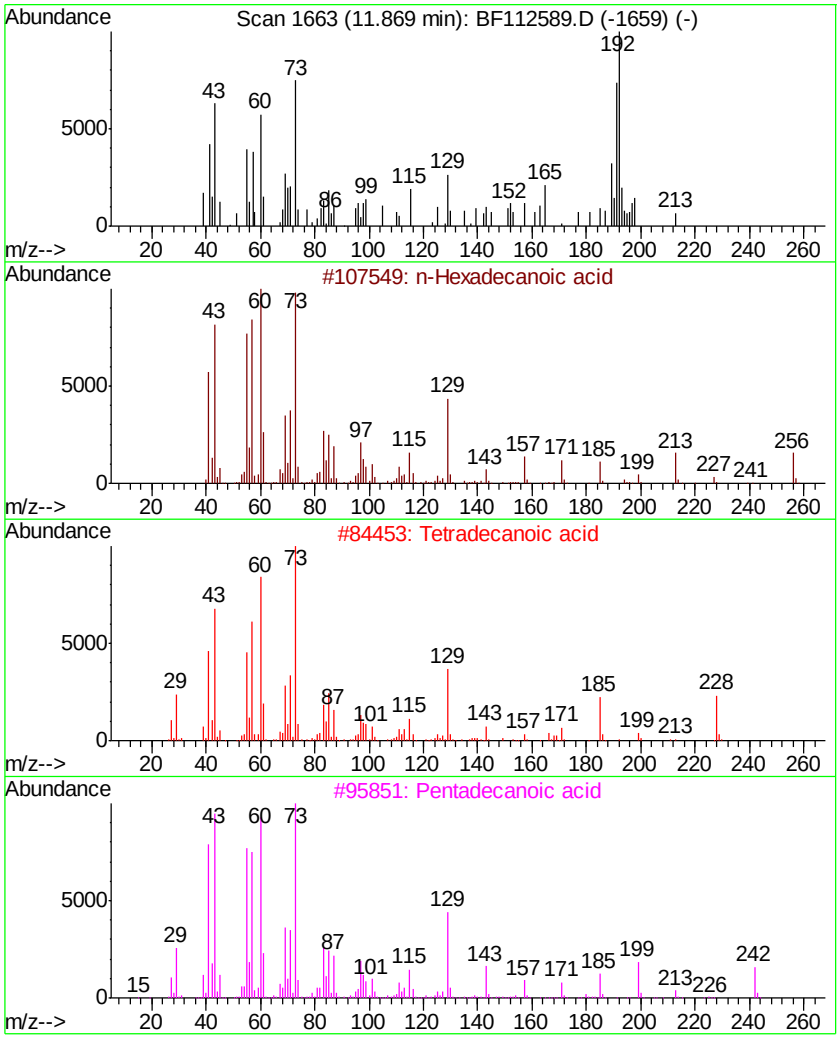
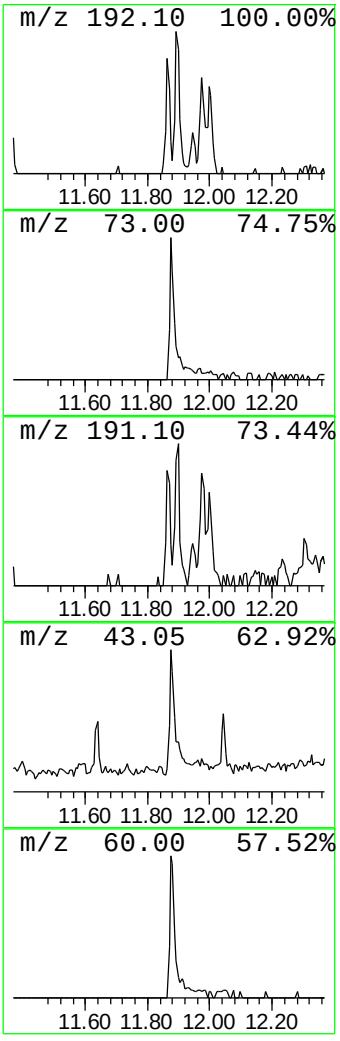
Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	3.33 ng	185696	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Dodecanoic acid	200	C12H24O2	000143-07-7	70
5	Tridecanoic acid	214	C13H26O2	000638-53-9	59





Library Search Compound Report

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Misc :
ALS Vial : 13 Sample Multiplier: 1

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

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

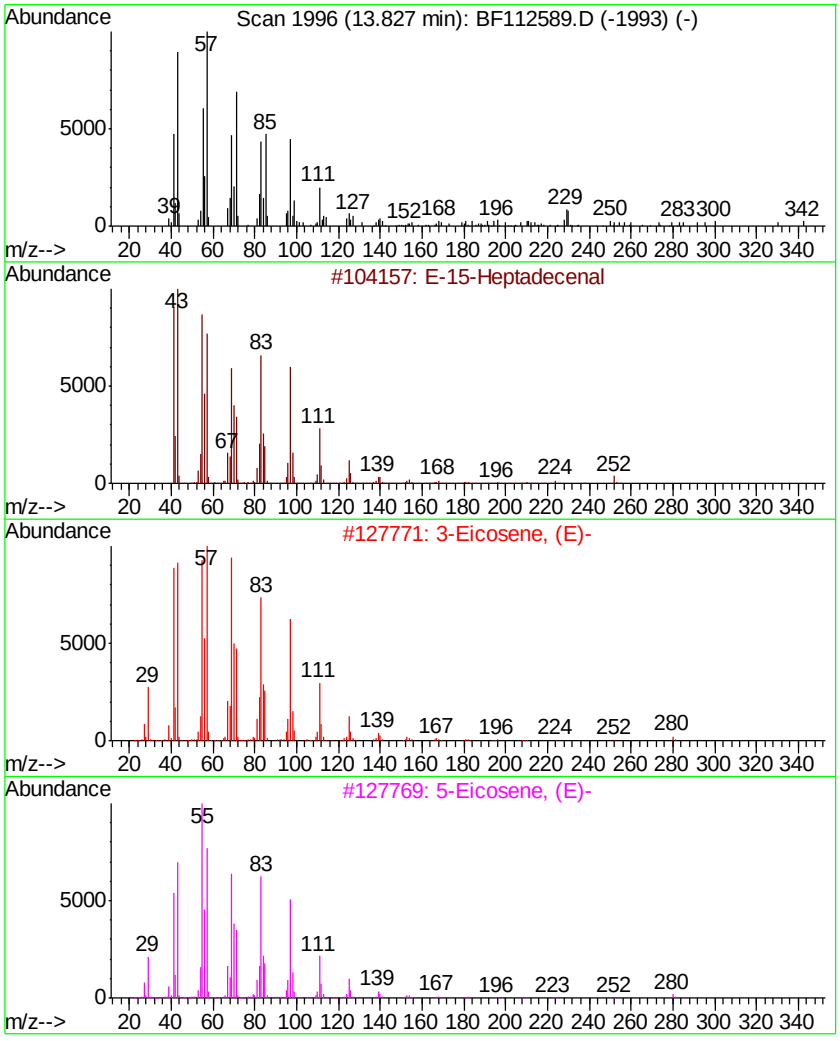
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

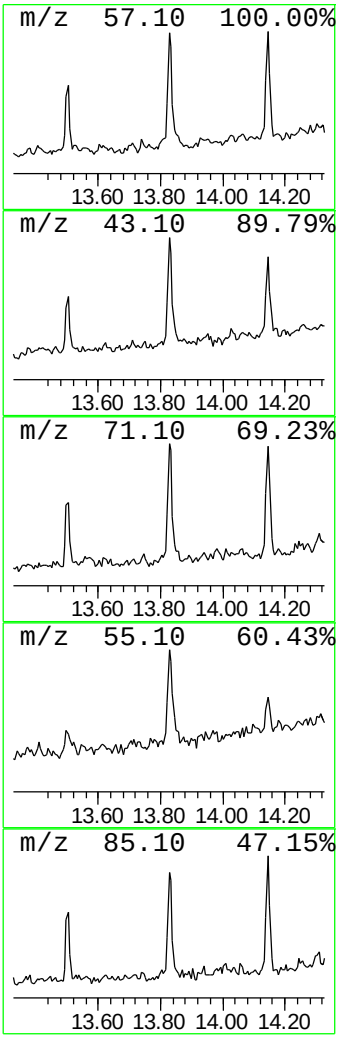
****

Peak Number 4 E-15-Heptadecenal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	4.15 ng	182835	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	86
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	83
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	80
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	64
5	Cyclotetradecane	196	C14H28	000295-17-0	59





Library Search Compound Report

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

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

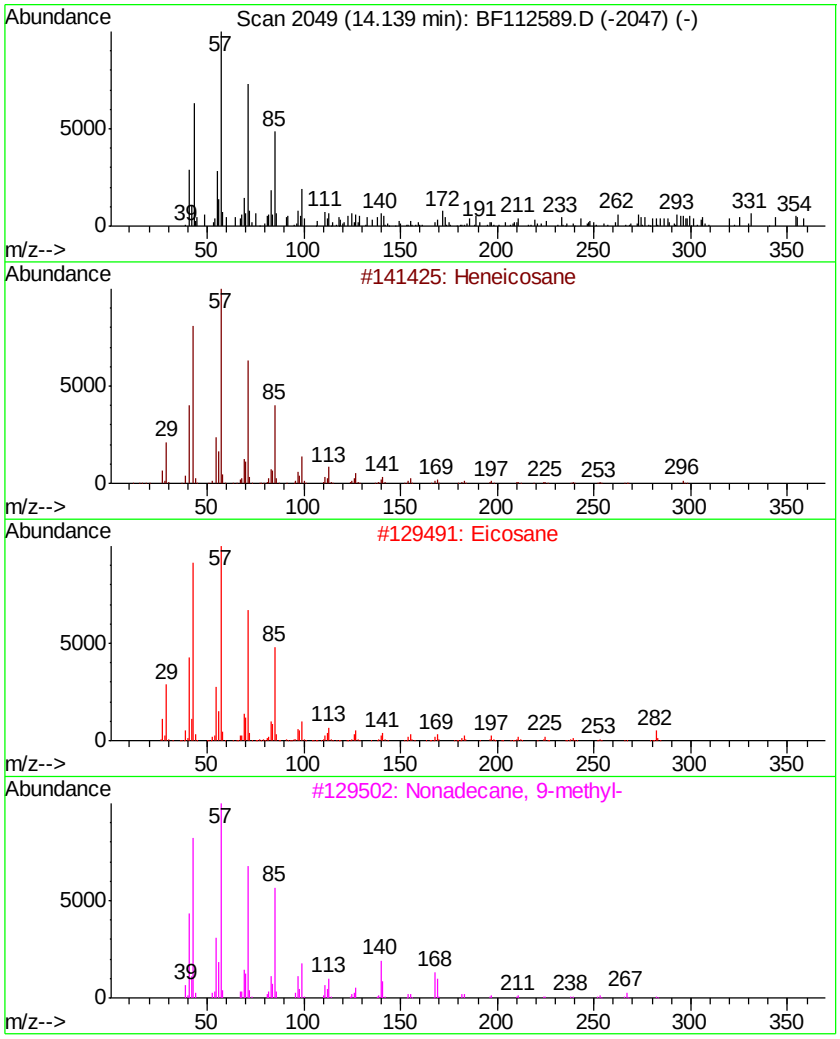
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

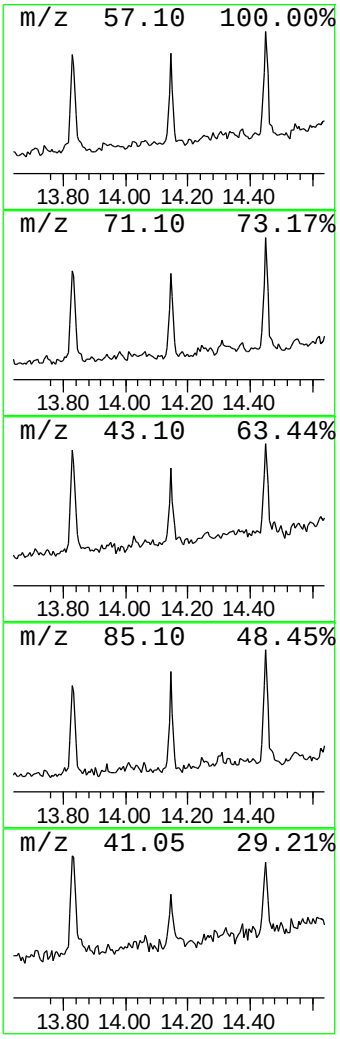
****

Peak Number 5 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.14	2.11 ng	92852	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	96
2	Eicosane	282	C20H42	000112-95-8	93
3	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	93
4	Pentadecane	212	C15H32	000629-62-9	90
5	Triacontane	422	C30H62	000638-68-6	87





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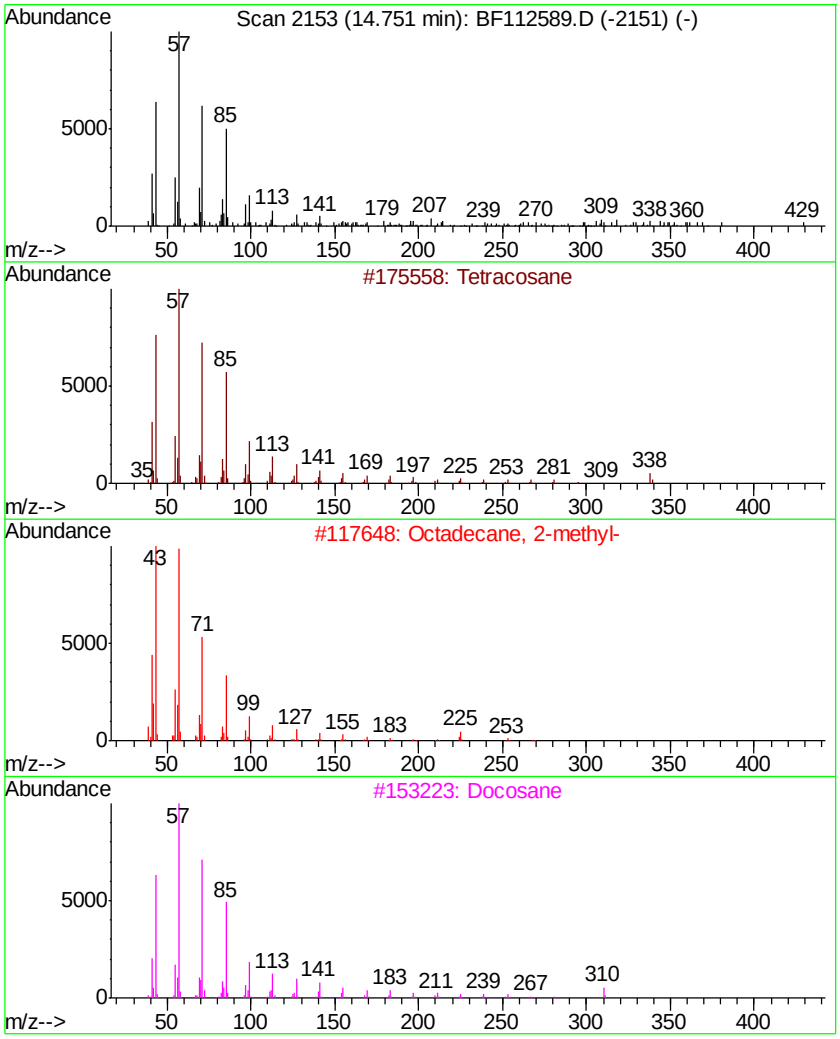
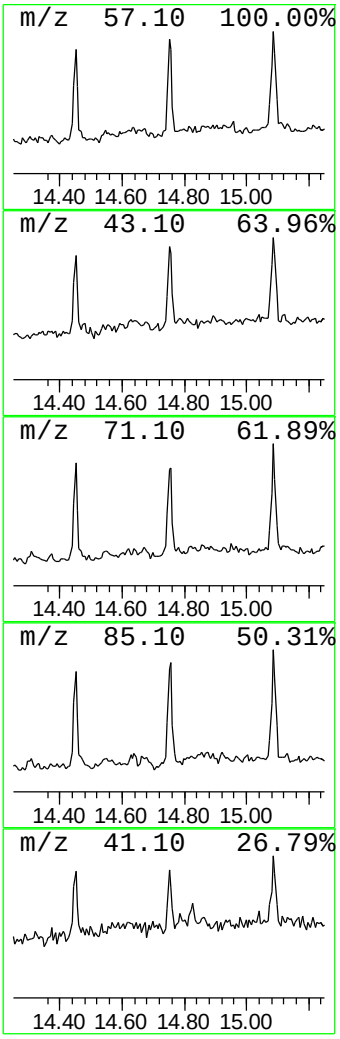
****

Peak Number 7 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	2.30 ng	101353	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	93
2	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
3	Docosane	310	C22H46	000629-97-0	91
4	Octadecane	254	C18H38	000593-45-3	87
5	Heneicosane	296	C21H44	000629-94-7	87





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

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

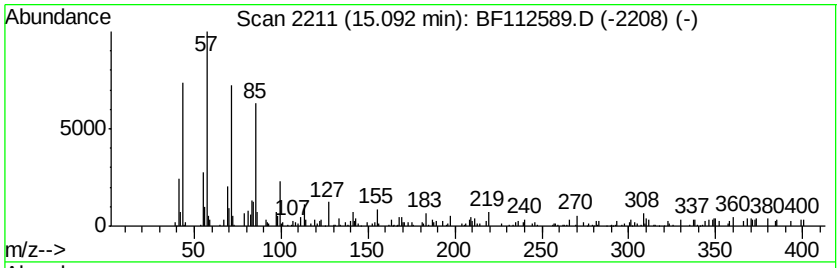
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

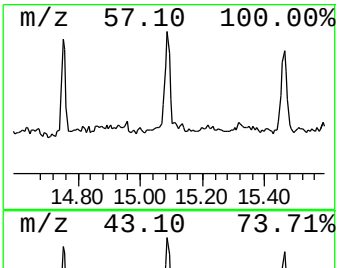
****

Peak Number 8 Pentadecane, 8-hexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	4.04 ng	128525	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90
2	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	90
3	2-Bromotetradecane	276	C14H29Br	074036-95-6	86
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
5	10-Methylnonadecane	282	C20H42	056862-62-5	86





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_F
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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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.61	6.61	39.9	ng	1301360	1	6.83	652136	20.0
n-Hexadecanoic acid	11.87	3.3	ng	185696	4	11.36	1114410	20.0
E-15-Heptadecenal	13.83	4.2	ng	182835	5	14.01	881453	20.0
Heneicosane	14.14	2.1	ng	92852	5	14.01	881453	20.0
Tetracosane	14.75	2.3	ng	101353	5	14.01	881453	20.0
Pentadecane, 8-he...	15.09	4.0	ng	128525	6	15.49	635674	20.0